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User's Guide for WASTOX, a Framework for Modeling the Fate of Toxic Chemicals in Aquatic Environments. Part 1. Exposure Concentration

Manhattan Coll., Bronx, NY

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Part 1: Exposure Concentration

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16. ABSTRACT

A computer program, WASTOX, is described as a technique for modeling the fate of toxic chemicals discharged into natural water systems. WASTOX is a batch-oriented program that solves the mass balance equations to define fate of toxic chemicals in aquatic environments. The report documents the exposure concentration component of the program, which analyzes the time-variable or steady-state, physical-chemical behavior of chemicals. The model is generally applicable to all types of water bodies.

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PART 1: EXPOSURE CONCENTRATION

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The WASTOX computer code has been tested against other computer programs to verify its computational accuracy. Nevertheless, errors are possible. The EPA assumes no liability for either misuse of the model or errors in the code. The user should verify the code before using it.

FOREWORD

The protection of estuarine and freshwater ecosystems from damage caused by toxic organic pollutants requires that regulations restricting the introduction of these compounds into the environment be formulated on a sound scientific basis. Accurate information describing the potential exposure of indigenous organisms and their communities to these toxic chemicals under varying conditions is required. The Environmental Research Laboratory, Gulf Breeze, contributes to this information through research programs aimed at determining:

- the effects of toxic organic pollutants on individual species, communities of organisms, and ecosystem processes.
- the fate and transport of toxic organics in the ecosystem.
- the application of methodologies which integrate fate and effects information to predict enviromental hazard.

The magnitude and significance of chemical contamination of aquatic environments are increasingly evident. The potential persistence and possible accumulation of those chemicals in aquatic food chains means that the impact on the health and activities of man is more direct. Therefore, the ability to predict exposure concentration, bioaccumulation, and chronic exposure is critical to our efforts in hazard assessment. Mathematical models provide a basis for quantifying the inter-relationships among the various physical, chemical, and biological variables that affect the fate, transport, and bioaccumulation of toxic chemicals. They also provide a mechanism for extrapolating laboratory information to the environment and a rationale and conceptually relevant basis for decisionmaking.

The modeling framework WASTOX described in this manual permits the user to examine the transport of a toxic chemical dissolved in water or sorbed to sediments, its transfer from one envioronmental medium (air, water, sediment, biological tissue) to another, and its reactivity relative to the processes of biodegradation, hydrolysis, photolysis, and oxidation. (Part I deals with the exposure concentration component of the WASTOX model. Part II will describe a food chain bioaccumulation model, and Part III will relate exposure and bioaccumulation to toxic effects.)

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ABSTRACT

A computer program was developed for modeling the fate of toxic chemicals that are discharged to natural water systems. The program permits the user to model the water and sediment transport in a natural water system and the movement and decay of chemicals discharged to that system. Either the equilibrium distribution of chemicals continually discharged to the system or the concentrations in the system as a function of time may be computed. From one to three types of solids may be considered.

The reaction of the chemical and its transfer among phases are computed from specified characteristics of the chemical and environmental parameters of the system. The processes considered include photolysis, hydrolysis, biodegradation, volatilization and adsorption. Adsorption to the solids types included in the model is described as a local equilibrium process defined by a partition coefficient and the local solids concentration. All other processes are defined in terms of reaction rates.

WASTOX does not explicitly specify each of the transport processes that may affect the chemical or solids. Transport is considered either as an advective process defined by a flow or a mixing process defined by a dispersion or exhange. Specification of separate transport processes is made by the user by defining up to nine sets of flows and dispersions (termed fields). Each field is applied to either dissolved chemical or adsorbed chemical and solids, or both. For example, dispersion within the stationary sediment is limited to dissolved chemical; therefore a field of dispersions would be specified by the user and applied only to this component. The user of such a non-specific transport structure permits construction of models consistent with the understanding of the particular natural water system and the question being addressed.

WASTOX is sufficiently general to be applied to all types of natural water systems. It has been successfully applied to the James River Estuary, the Great Lakes, and the U.S. Environmental Protection Agency (EPA) experimental stream channels at Monticello, Minnesota.

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WASTOX was developed from a version of WASP used at Manhattan College and we acknowledge the efforts of those involved in WASP's development, particularly James Fitzpatrick of HydroQual, Inc. and Gregory Clemens of Manhattan College.

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SECTION 1

INTRODUCTION

In problems concerning toxic chemicals in aquatic environments, one of two regulatory questions is generally posed: (1) what is the maximum allowable discharge of a toxic chemical to a water system for a specified use of the system, and (2) how long will it take a contaminated natural water system to recover to some specified level? The former question acknowledges that chemical discharges are an unavoidable component of our technological society and addresses the issue of allocation of the wasteload capacity of a natural water system relative to a given use and associated criteria. For this case, the relevant chemical concentration for regulatory evaluation is the equilibrium or steady-state value. The latter question deals with an unregulated or accidental discharge whose adverse effects must be assessed in terms of future use of the contaminated system. For this case, the time dependent behavior of the chemical in the system must be estimated.

To address these questions the physical, chemical and biological characteristics of both the system and the chemical must be specified. These characteristics determine the fate of the chemical by defining the rates of transport, transfer, and reaction.

Transport is the physical movement of the chemical caused by the net advective movement of water, mixing, and the scouring and deposition of solids to which the chemical may be adsorbed. It is specified by the flow and dispension characteristics of the natural water system and the settling velocity and resuspension rate of the solids in the system.

Transfer is the movement of the chemical between the air, water, and solid phases of the system. It includes the processes of volatilization, adsorption, and bioconcentration-bioaccumulation.

Reaction is the transformation or degradation of the chemical. It includes biodegradation and the chemical reaction processes of photolysis - hydrolysis, and oxidation.

The characteristics of the chemical are determined by a laboratory evaluation of the transfer and reaction processes. These controlled experiments provide data from which the kinetics of reaction and transfer may be determined. This information may then be combined with a theoretical development for transport to form an analysis framework or mathematical model. The model is the means by which the questions posed previously may be answered for a specific water body.

As part of projects to determine the fate of toxic chemicals in estuaries and the Great Lakes, a general model has been developed. This model calculates the time-variable or steady-state concentrations of dissolved and adsorbed chemical in any natural water system. It is named WASTOX, an acronym for Water quality Analysis Simulation of TOXics, and was developed from the Hydroscience, Inc. water quality model WASP (20).

The equations that comprise the model are developed using the principle of mass conservation, including the inputs with the transport, transfer and reactions components. The general expression for the mass balance equation about a specified volume, V, is:

$$V \frac{dc}{dt} = J + \Sigma R + \Sigma T + \Sigma W \qquad (1\text{-}1)$$

in which

c = concentration of the chemical
J = transport through the system
R = reactions within the system
T = transfer from one phase to another
W = inputs

Equation (1-1) describes the mass rate of change of the chemical due to the net effect of the various fluxes and transformations. The purpose of expressing the transfer rate (T), distinct from the transport (J) and reaction (R), is to provide a basis for the development of the equations, which describe more fully the relevant phenomena. The transport, reaction and transfer terms may be positive or negative depending on the direction of kinetic routes.

To obtain a time variable solution of Equation (1-1), it is necessary to employ numerical methods. The approach used is to approximate the spatial derivatives that define the transport component of the equation and the temporal derivative with difference expressions. This is equivalent to separating the natural water system being modeled into a series of completely-mixed sections. The size of the sections is controlled by the time step constraints imposed by the stability limitations of the numerical scheme and the extent of spatial resolution desired.

To obtain the steady state solution of Equation (1-1) difference expressions are used to approximate the spatial derivatives and the time derivative, dc/dt is set equal to zero. The resulting set of simultaneous algebraic equations are solved using the Gaussian Elimination technique.

The model is general in nature. The natural water system under study may be sectioned or segmented as the user chooses. Transport is defined by dispersion coefficients and flows that are specified in a series of fields that are individually applied to both the particulate and dissolved chemical (e.g., hydrodynamic flow), the particulate chemical only (e.g., resuspension), or the dissolved chemical only (e.g., interstitial water diffusion).

The reaction and transfer components are computed in a single subroutine separate from the transport and integration computations. This kinetic subroutine has been developed to provide the user with the capability to alter the transfer and reaction formulations or to add additional kinetic processes.

The kinetic subroutine returns to the main program that portion of the time derivative $(\frac{dc}{dt})$ contributed by the transfer and reaction components. Changes may be made by adding terms to this derivative computation. The variables that define a specific kinetic process are transmitted to the kinetic subroutine through a segment dependent array of parameters and an array of constants. These may be altered by the user through respecification of the equivalence statements in the kinetic subroutine. A copy of the present kinetic structure is included in Appendix A.

The simple Euler-Cauchy method is used for the integration of the time derivative. Results are filed at a user specified print interval and displayed at the conclusion of the program execution.

SECTION 2
FUNDAMENTAL EQUATIONS

One of the most distinguishing characteristics of toxic substances is the partitioning between dissolved and particulate components. Thus equations are developed for each of these components and in addition for those solids which provide sites for the adsorption of the substance. The analysis involves therefore, the solution of at least three simultaneous equations, describing the concentration of the various components in the water column. Furthermore, for interaction with the bed, additional sets of equations are developed to account for distribution in the benthal layer and its effect on water column concentrations. Given these concentrations, the dissolved and the particulate in the water column and in the bed, the distribution through the food chain is then analyzed.

2.1 WATER COLUMN

Consider the concentration, c, to be the dissolved component of the chemical in water. It interacts with the particulate concentration, p, through an adsorption-desorption reaction with the solids. The particulate concentration is defined as:

$$p = rm \tag{1}$$

p = particulate concentration M/L^3
r = mass of chemical/unit of solids mass M/M
m = concentration of the solids M/L^3

The equations governing the distribution of the dissolved and particulate components in a natural water system may be written as follows:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(E_x \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(E_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(E_z \frac{\partial c}{\partial z}\right) - \frac{\partial}{\partial x} u_x c - \frac{\partial}{\partial y} u_y c - \frac{\partial}{\partial z} u_z c - K_o mc + K_2 p \pm S_1(x,y,z,t) \tag{2}$$

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x}\left(E_x \frac{\partial p}{\partial x}\right) + \frac{\partial}{\partial y}\left(E_y \frac{\partial p}{\partial y}\right) + \frac{\partial}{\partial z}\left(E_z \frac{\partial p}{\partial z}\right) - \frac{\partial}{\partial x} u_x p - \frac{\partial}{\partial y} u_y p - \frac{\partial}{\partial z} u_z p + \frac{\partial}{\partial z} w_s p + K_o mp - K_2 p \pm S_2(x,y,z,t) \tag{3}$$

in which

c = concentration of the dissolved component $[M/L^3]$
E = dispersion coefficient $[L^2/T]$
u = velocity $[L/T]$
w_s = settling velocity of the particulates $[L/T]$
K_o = adsorption coefficient $[L^3/(M \cdot T)]$
K_2 = desorption coefficient $[T^{-1}]$
x,y,z = coordinate directions
t = time $[T]$
S = sources and sinks of the component due to reactions and phase transfers

The first three terms in each equation represent dispersion or mixing due to temporal and spatial velocity gradients and density differences within the natural water system. The next three terms represent the longitudinal, lateral and vertical advection, respectively. The seventh term in equation (3) accounts for the vertical advection of the particulate component due to settling. The following two terms define the rates of adsorption and desorption, respectively. The last term accounts for the chemical and biological reactions and volatilization that may produce or degrade the component.

The vertical boundary conditions are assigned at the air-water and water-bed interfaces, at which concentration and flux conditions are specified. The flux may be negative or positive, representing net deposition or scour at the bed, respectively, or gas-liquid exchange at the air-water surface. An additional source due to precipitation may be effective under certain conditions.

Note that since the distributions of the dissolved and particulate components depend on the concentration of the solids, m, an expression equivalent to Eqs. 2 and 3 must be written for the distribution of the solids:

$$\frac{\partial m}{\partial t} = \frac{\partial}{\partial x}\left(E_x \frac{\partial m}{\partial x}\right) + \frac{\partial}{\partial y}\left(E_y \frac{\partial m}{\partial y}\right) \frac{\partial}{\partial z}\left(E_z \frac{\partial m}{\partial z}\right) - \frac{\partial}{\partial x} u_x m - \frac{\partial}{\partial y} u_y m - \frac{\partial}{\partial z} u_z m + \frac{\partial}{\partial z} w_s m \tag{4}$$

If more than one solid is considered, i.e., several solid classes, then two additional equations must be included for each additional component to describe the particulate and solids concentrations.

The particulate and dissolved concentrations can be summed to yield the total concentration of chemical, c_T:

$$c_T = \theta c + p \tag{5}$$

or if several solids types are considered:

$$c_T = \theta c + \sum_{i=1}^{n} p_i \tag{6}$$

where θ is porosity (water volume/total volume).
The particulate concentration is related to the concentration of solids, m, as shown by equation (1):

$$p = rm$$

Equation (6) may therefore be written as:

$$c_T = \theta c + \sum_{i=1}^{n} r_i m_i \tag{7}$$

If adsorption equilibrium is assumed then the relationship between the dissolved chemical concentration and the mass concentration of adsorbed chemical, r (M chemical/M solid), is specified by the sorption isotherm. For many chemicals in natural water systems the isotherm is linear and is expressed in terms of a partition coefficient ¶ (L^3/M):

$$r = \P c \tag{8}$$

Combining equations (7) and (8), the total concentration may be expressed as:

$$c_T = c[\theta + \Sigma \P_i m_i] \tag{9}$$

The fraction of total chemical that is dissolved, f_d, may then be written as:

$$f_p = \frac{c}{c_T} = \frac{1}{\theta + \Sigma \P_i m_i} \tag{10}$$

Similarly, the fraction of total chemical adsorbed to a particular solids type j, f_{pj}, is given as:

$$f_{p_j} = \frac{p_j}{c_T} = \frac{\pi_j m_j}{\theta + \Sigma \pi_i m_i} \tag{11}$$

It is evident from equations (10) and (11) that the distribution of the dissolved and particulate components may be determined directly from the distributions of total chemical concentration and solids concentration. A reduction in the number of equations included in the modeling framework is realized since only one equation for the chemical and one for each solids type is required whereas previously an equation for dissolved chemical and two equations for each solids type, one for particulate chemical and one for the solids, were required.

An equation describing the distribution of total chemical is obtained by summing the equations for dissolved and particulate (equations (2) and (3)):

$$\frac{\partial c_T}{\partial t} = \frac{\partial}{\partial x} (E_x \frac{\partial c_T}{\partial x}) + \frac{\partial}{\partial y} (E_y \frac{\partial c_T}{\partial y}) + \frac{\partial}{\partial z} (E_z \frac{\partial c_T}{\partial z})$$

$$- \frac{\partial u_x c_T}{\partial x} - \frac{\partial u_y c_T}{\partial y} - \frac{\partial u_z c_T}{\partial z} + \frac{\partial}{\partial z} w_s (f_{p_i} c_T) \pm S \tag{12}$$

2.2 SEDIMENT BED

The transport components of the bed may include a longitudinal advection and a vertical dispersion or mixing. The advective component of transport in the bed is significant in rivers and estuaries where it is induced by shearing stress of the overlying flowing water, with which it is in contact. The horizontal velocity of the bed is a maximum at the water interface and diminishes in depth to a point at which the bed may be regarded as stationary. The vertical dispersion follows a similar pattern. A mass balance about an elemental volume within the bed results in the following equation defining the solids distribution:

$$\frac{\partial m}{\partial t} = \frac{\partial}{\partial z} (\varepsilon(x) \frac{\partial}{\partial z}) + \frac{u(z)}{B(x)} \frac{\partial Bm}{\partial x} \tag{13}$$

in which

ε = vertical mixing coefficient (L^2/T)
u = horizontal velocity (L/T)
B = width of the bed (L)

The boundary condition in the vertical planes are specified at the water-bed interface and at that depth of zero horizontal velocity, which is the interface between the transport layer and the stationary bed. The former is the net flux, J, due to the settling of suspended solids from the overlying water and the resuspension from the transport or surface layer of the bed:

$$J_b = w_s m_w - w_u m_b \qquad (14)$$

in which m_b is the concentration of particles in the sediment layer, m_w is the concentration of particles in the water column and w_u is the entrainment velocity of these sediment particles across the interface. A net flux from the water to the sediment layer implies that the mean settling is greater than the resuspension of particles and conversely a net flux from the sediment layer to the water stipulates that uplift is greater than settling. The net effect of this flux is a change in the elevation of the water-bed interface, which rises or falls depending on the relative magnitude of the two terms in the above equation. A volumetric change results in the bed that must be taken into account in the mass balance.

Assuming vertical uniformity of solids concentration in the surface bed layer, a mass balance results in the following equation defining the solids distribution:

$$\frac{\partial V m_b}{\partial t} = w_s m_w A - w_u m_b A + \frac{Vu}{B(x)} \frac{\partial}{\partial x} (B m_b) \qquad (15)$$

in which V is the bed volume and A is the surface area of the bed. The vertical dispersion term of equation (14) does not appear because by definition there is no vertical solids gradient. It is replaced by the flux condition at the boundary.

Replacing the volume term by the product of the length and cross-sectional area, A_c, of the layer, expanding the left side of the equation, and dividing through by the cross-sectional area:

$$\frac{\partial m_b}{\partial t} + \frac{m_b}{A_c}\frac{\partial A_c}{\partial t} = \frac{w_s}{h} m_w - \frac{w_s}{h} m_b + \frac{u}{B}\frac{\partial}{\partial x}(Bm_b) \qquad (16)$$

in which h = depth of the layer. Assuming the width of the bed is constant in time:

$$\frac{1}{A_c}\frac{\partial A_c}{\partial t} = \frac{1}{h}\frac{dh}{dt} = \frac{w_d}{h} \qquad (17)$$

$\frac{dh}{dt} = w_d$ = the rate of change of the bed elevation

The rate of change of the bed elevation is referred to as a sedimentation velocity. It may be envisioned as the velocity at which the water-bed interface approaches the stationary bed if erosion is predominant or at which the interface moves away from that datum if settling is the significant term.

Assuming the concentration of the bed, m_b, is approximately constant, the above reduces to, under steady-state:

$$0 = \frac{w_s m_w}{h} - \frac{m_b}{h}(w_u + w_d) + u m_b b \qquad (18)$$

in which

$$b = \frac{1}{B}\frac{dB}{dx}$$

For a stationary bed u is zero and the last term in equation (18) drops out. Intrepreting the bed elevation change as described, the flux about a lower bed layer is:

$$w_d m_b = w_{d\ell} m_s \qquad (19)$$

in which

$w_{d\ell}$ = sedimentation velocity in the lower bed layer

m_s = average concentration of the solids in the lower bed layer.

A mass balance on particulate chemical in the bed follows that for solids directly. For dissolved chemical a flux at the sediment-water interface, J_d, specified in terms of a dispersion coefficient, E, is incorporated:

$$J_d = -E \frac{\partial c}{\partial z} \Big|_{z=\text{sediment-water interface}} \tag{20}$$

Assuming a constant concentration of solids within a layer of depth H adjacent to the water column, the equation describing the distribution of total chemical in that layer is:

$$\frac{\partial c_{T_b}}{\partial t} = \frac{w_s}{h} f_p c_{T_w} - \frac{f_p}{h} (w_u + w_d) c_{T_b} + ubc_{T_b} - \frac{EA}{\ell} (f_{d_b} c_{T_b} - f_{d_w} c_{T_w}) \tag{21}$$

where ℓ is the average depth of the surface bed layer and the adjacent water column layer. Dispersion of dissolved chemical between the surface and lower bed layers adds a term to equation (21) that is analogous to that for dispersion with the water column. Figure 1 illustrates the components of equation (21).

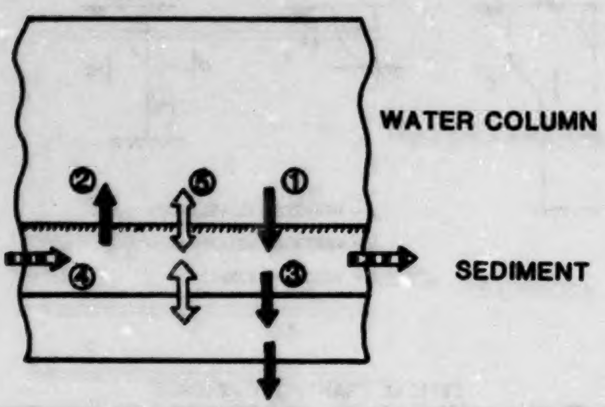
2.3 APPLICATION TO A SPECIFIC WATER BODY

The water column and bed equations are general in nature and are usually simplified when applied to a specific water body. Typical transport regimes for the various types of water bodies are shown in Figure 2. In rivers advection is dominant and the water column is fairly well-mixed vertically and laterally. Therefore, the lateral and vertical spatial derivatives in equation (12) may be dropped reducing the equation to a single dimension. Settling is included as a boundary condition at the water-bed interface.

In estuaries vertical concentration gradients may be important and only the lateral spatial derivative is dropped. Equation (12) is therefore reduced to a two-dimensional equation.

In lakes, the bed equation is generally simplified because the low velocities do not cause significant horizontal movement of the bed. The horizontal velocity term in equation (21) is dropped reducing the equation to a single dimension.

Further simplifications are sometimes made depending on the space and time scales of interest. Several of these are illustrated in the applications of WASTOX presented in Section 6.



PROCESS	MASS FLUX TERM
① DEPOSITION OF SOLIDS	$\frac{W_s}{h} f_p C_{T_w}$
② SCOURING OF SOLIDS	$\frac{W_u}{h} f_p C_{T_b}$
③ NET SEDIMENTATION	$\frac{W_d}{h} f_p C_{T_b}$
④ HORIZONTAL BED MOVEMENT	$\frac{u}{B} \frac{d}{dx} (B C_{T_b})$
⑤ DIFFUSION OF DISSOLVED CHEMICAL	$\frac{EA}{\ell} (f_{d_b} C_{T_b} - f_{d_w} C_{T_w})$

FIGURE 1. FLUXES OF TOXIC CHEMICAL ASSOCIATED WITH THE BED

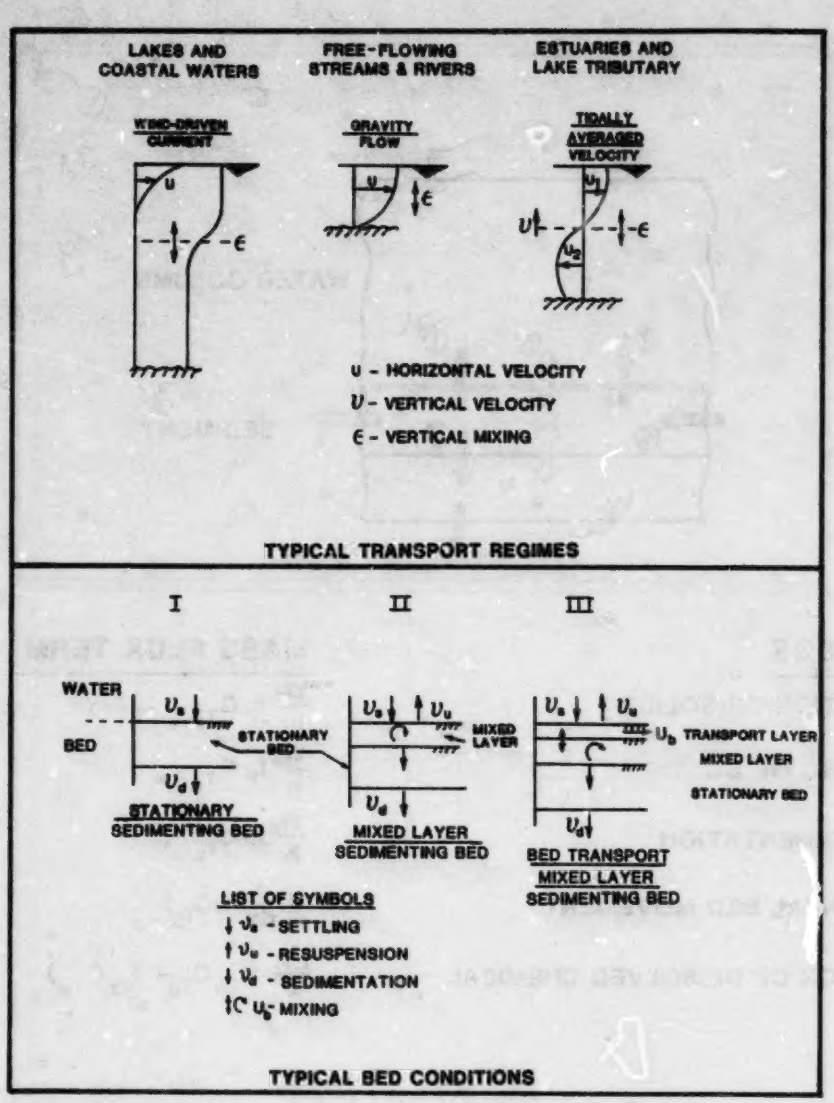

LAKES AND COASTAL WATERS
FREE-FLOWING STREAMS & RIVERS
ESTUARIES AND LAKE TRIBUTARY
WIND-DRIVEN CURRENT
GRAVITY FLOW
TIDALLY AVERAGED VELOCITY
u
ε
v
u_1
u_2
u - HORIZONTAL VELOCITY
v - VERTICAL VELOCITY
ε - VERTICAL MIXING
TYPICAL TRANSPORT REGIMES
I
II
III
WATER
BED
v_s
v_u
v_d
U_b
STATIONARY BED
MIXED LAYER
TRANSPORT LAYER
MIXED LAYER
STATIONARY BED
STATIONARY SEDIMENTING BED
MIXED LAYER SEDIMENTING BED
BED TRANSPORT MIXED LAYER SEDIMENTING BED
LIST OF SYMBOLS
v_s - SETTLING
v_u - RESUSPENSION
v_d - SEDIMENTATION
U_b - MIXING
TYPICAL BED CONDITIONS

FIGURE 2. TYPICAL CHARACTERISTICS OF NATURAL WATER SYSTEMS: (a) Typical transport regimes, b) Typical bed conditions

SECTION 3

MODELING FRAMEWORK

3.1 FINITE DIFFERENCE APPROXIMATION

WASTOX is in essence a computer program that solves the equations presented in Section 2. The solution of these equations is accomplished using finite difference approximations to the spatial derivatives in identical fashion to the Water Quality Analysis Simulation Program (WASP) (20). The water body is divided into completely-mixed segments in which the concentrations of total chemical and solids are calculated by the finite-difference approximations of their mass balance equations. For total chemical the equation for segment i is as follows:

$$\begin{aligned} V_i \frac{dc_i}{dt} = {} & \sum_j Q_{j,i} c_j - \sum_k Q_{i,k} c_i + \sum_j \frac{E_{i,j} A_{i,j}}{L_{i,j}} (c_j - c_i) \\ & - w_{s_{i,\ell}} A_{i,\ell} f_{p_i} c_i + w_{u_{\ell,i}} A_{i,\ell} f_{p_\ell} c_\ell + \frac{E_{i,\ell} A_{i,\ell}}{L_{i,\ell}} (f_{d_\ell} c_\ell - f_{d_i} c_i) \pm S \end{aligned} \tag{22}$$

where

V_i = volume of segment i

c_i = total chemical concentration in segment i (subscript t dropped for convenience)

$Q_{j,i}$ = hydrodynamic flow from segment j to segment i

$E_{i,j}$ = dispersion coefficient between segment i and segment j

$A_{i,j}$ = cross-sectional area between segments i and j

$L_{i,j}$ = characteristic length or mixing length of segments i and j

$$L_{i,j} = \frac{L_i + L_j}{2}$$

$w_{s_{i,\ell}}$ = settling velocity of particulates from segment i to segment ℓ

$w_{u_{\ell,i}}$ = resuspension velocity of particulates from segment ℓ to segment i (included only if the i,ℓ interface is a water-bed interface)

(Note: $E_{i,\ell}$ is fundamentally the product of porosity and the dispersion coefficient and would be included only if i,ℓ is a water-bed or bed-bed interface)

WASTOX applies equation (22) to each of the segments the water body is divided into. However, the explicit separation of hydrodynamic flow, settling, resuspension, sedimentation, water column dispersion and interstitial water diffusion indicated by equation (22) is not formalized in the computer code. The program considers all transport as either a flow or a dispersion. Including different transport processes is accomplished through the use of multiple sets of flows and dispersions, termed fields. These fields are applied to either dissolved chemical or adsorbed chemical and solids, or both. For example, dispersion within the bed is limited to dissolved chemical and a separate grouping or field of dispersions is inputted by the user and applied only to this component. The type and number of transport processes included is the decision of the user based on the fundamental processes indicated in Section 2, the characteristics of the water body being modeled, and the particular segment, i.e., water column or sediment, at or away from the water-bed interface.

For time variable solutions equation (22) is solved using a forward difference approximation for the time derivative. The concentration at time n+1 is equal to the concentration at time n plus the derivative evaluated at time n multiplied by the time step, Δt;

$$C_i^{n+1} = c_i^n + \left(\frac{dc_i^n}{dt}\right)\Delta t \qquad (23)$$

To maintain a stable solution for the numerical scheme the size of the time step must be restricted. The stability criteria and numerical error associated with the solution scheme are the same as for WASP (20).

For computational stability a necessary condition is that

$$\Delta t \leq \text{Min} \left(\frac{V_i}{\sum_j Q_{i,j} + \sum_j R_{i,j} + K_i V_i}\right) \qquad (24)$$

where

$$R_{i,j} = \text{exchange coefficient} = \frac{E_{ij} A_{ij}}{L_{i,j}} \qquad (25)$$

K_i = reaction rate of the chemical

However, since K is, for many applications, non-linear and time-dependent itself, and therefore may be difficult to evaluate, the following criteria may be used for choosing the integration step-size

$$\Delta t < \text{Min} \left(\frac{V_i}{\sum_j Q_{ij} + \sum_j R_{ij}} \right)$$

providing that

$$\text{Max} \, (K_i V_i) << \sum_j Q_{ij} + \sum_j R_{ij}.$$

The use of the completely mixed finite segment approximation in conjunction with a backward difference spatial approximation, introduces a numerical error (sometimes referred to as numerical or pseudo-dispersion) into the model. The extent of this effect is given by

$$E_{num} = \frac{u\Delta x}{2}$$

where E_{num} is the numerical error expressed as a pseudo-dispersion coefficient and Δx is the length of the segment in the direction of the velocity u. For some applications, especially in well mixed estuaries, where the time scale of importance is on the order of days to seasons rather than hours, and where u is the net advective freshwater velocity (usually small), the effect of the numerical error, E_{num}, is generally not significant.

For steady state solutions the time derivative in Equation (22) is set equal to zero yielding an algebraic equation for each segment. This set of simultaneous equations may be written as:

$$[A](c) = (w) \qquad (26)$$

where [A] is an nxn matrix (n = number of segments) including the transport and reaction terms of Equation (22), (c) is the vector of segment concentrations, and (w) is the vector of mass loadings to each segment. The steady state concentrations can be obtained by inversion of the [A] matrix, i.e.,

$$(c) = [A]^{-1}(w) \qquad (27)$$

Direct inversion of the [A] matrix is valid only if the reaction terms included in the model are linear, as they are in WASTOX. If non-linear reactions were included an iterative solution scheme would have to be used.

3.2 KINETICS

Kinetic expressions that define the time rate of transfer of chemical between phases and transformation to degradation products comprise the terms S_1 and S_2 in equations (2) and (3), respectively. The processes of volatilization, photolysis, chemical hydrolysis and microbial degradation are included.

3.2.1 Volatilization

The transfer of a volatile substance between air and water occurs when the concentration in one medium is not in equilibrium with the concentration in the other. The rate of transfer per unit area in each phase is proportional to the driving force, which is the partial pressure gradient in the gas phase and concentration gradient in the liquid phase. Under steady state conditions the unit transfer is:

$$j = K_L[c_{\ell i} - c_\ell] = K_G[c_g - c_{gi}] \tag{28}$$

The subscripts ℓ and g refer to the liquid and gas phases, respectively. $c_{\ell i}$ and c_{gi} are the concentrations at the air-water interface, c_ℓ and c_g are the bulk concentrations, and K_ℓ and K_g are the mass transfer coefficients between the interface and the bulk phase. Assume the concentrations are at equilibrium at the surface of contact between the two phases, i.e., $c_{gi} = Hc_{\ell i}$, in which "H" equals Henry's constant. Solving for $c_{\ell i}$ and substituting this expression into the flux equation yields:

$$j = k_\ell[c_g/H - c_\ell] = k_g[c_g - Hc_\ell] \tag{29}$$

in which

k_ℓ and k_g are the overall transfer coefficients

$$\frac{1}{k_\ell} = \frac{1}{K_L} + \frac{1}{HK_G} \tag{30a}$$

$$\frac{1}{k_g} = \frac{1}{K_G} + \frac{H}{K_L} \tag{30b}$$

For exchange between the atmosphere and natural water systems, the ratio of the liquid film coefficient, K_L, to the gas film coefficient, K_G, is in the range of 0.0001-0.005. Therefore for substances with Henry's constant greater than 10, the resistance to transfer is localized in the aqueous film and for Henry's constant less than 10^{-4}, in the gas film.

The gas phase concentration of most toxic chemicals is essentially zero and the flux may be written as:

$$j = k_\ell c_\ell \tag{31}$$

It is evident that to evaluate the transfer rate, k_ℓ, values for the liquid phase transfer coefficient, K_L, the gas phase transfer coefficient, K_G, and the Henry's constant, H, are required.

In the classic two-film theory of transfer (1), from which the above equations were derived, the transfer coefficients may be defined as:

$$K = \frac{D}{\delta} \tag{32}$$

ιν δηιΨη δ is the thickness of the diffusional or viscous layer and D is the molecular diffusivity of the chemical. Since the relationship applies to both air and water, the subscripts are omitted.

An approach based on the concept of surface renewal has been presented (2). The analysis, postulated on a random replacement of the elements at the interface, leads to a definition of the transfer coefficient as follows:

$$K = \sqrt{Dr} \tag{33}$$

in which r = rate of surface renewal. A definition of the renewal rate has been proposed (3) as the ratio of the intensity to the scale of turbulence in the vicinity of the interface. The vertical velocity fluctuation, $\bar{\nu}$, is representative of the intensity and the mixing length, ℓ, of the scale, and the renewal rate is the ratio of these:

$$r = \frac{\bar{\nu}}{\ell} \tag{34}$$

Surface renewal implies turbulent flow extending to the interface with no diffusional or viscous layer. It is applicable to the liquid phase of flowing waters such as streams and estuaries. For such systems the rate of surface renewal, r, has been shown (3) to be approximated by the ratio of the velocity, u, to the depth, h:

$$r = \frac{u}{h} \tag{35}$$

The depth, h, is the depth of the well-mixed layer, which is the total depth in streams and the depth of the surface layer in stratified estuaries. Substituting equation (35) into equation (33) yields:

$$K_L = \left(\frac{Du}{h}\right)^{1/2} \tag{36}$$

For more quiescent systems such as lakes, where surface renewal does not extend to the interface, a viscous sublayer exists. In these systems mass transfer is controlled by diffusion through the liquid and gas sublayers as indicated by equation (32). Because the structure of the sublayers is affected by the shearing action of winds on the water surface the transfer coefficients are related to wind activity.

The liquid mass transfer coefficient due to winds may be expressed as (4):

$$K_L = \left[\frac{D_L}{\nu_w}\right]^{2/3} \left[c_d \frac{\rho_a}{\rho_w}\right]^{1/2} \frac{W_{10}}{\lambda_L} \tag{37}$$

where

D_L = diffusion coefficient of the chemical in water

ν_w = viscosity of water

c_d = drag coefficient
ρ_a = density of air
ρ_w = density of water
W_{10} = wind velocity at 10 meters above the water surface
λ_L = coefficient related to the thickness of the liquid viscous sublayer

The gas term K_G is primarily affected by wind action and the structure of the diffusional sublayer in the interfacial region. By analogy to the liquid mass transfer coefficient relationship to winds, K_G is expressed as:

$$K_G = \left[\frac{D_G}{\nu_a}\right]^{2/3} \left[c_d \frac{\rho_a}{\rho_w}\right]^{1/2} \frac{W_{10}}{\lambda_G} \qquad (38)$$

where

D_G = diffusion coefficient of the chemical in the atmosphere
ν_a = viscosity of air
λ_G = coefficient related to the thickness of the gas viscous sublayer

The gas mass transfer coefficient for a flowing system like an estuary when there is no wind is undefined. It is estimated at 50-100 m/d by contrast to values in the order of 1000 m/d for large open water systems under moderate wind speeds.

Winds are most significant for open water bodies such as lakes and bays. Most flowing systems are sheltered and are only significantly affected by winds parallel to the longitudinal axis of the system. The lower portion of an estuary, i.e., the harbor area, is generally more open than the upstream area and winds may be significant to air-water transfer in these regions.

If the model is directed to stream or estuarine environments (flowing systems), the liquid mass transfer coefficient is specified by equation (36). Wind effects are not considered in specifying the gas phase mass transfer coefficient. It is set at a constant value of 100 m/d, acknowledging that this may not be valid for harbor regions or systems subjected to strong winds along their main axis. For lake and ocean environments the mass transfer coefficients are calculated by equations (37) and (38).

3.2.2 Photolysis

Photodecomposition (photolysis) is the transformation or degradation of a compound that results directly from the adsorption of light energy. It is a function of the quantity and wavelength distribution of incident light, the light absorption characteristics of the compound and the efficiency at which adsorbed light produces a chemical reaction. Photolysis is classified into two types that are defined by the mechanism of energy absorption. Direct photolysis is the result of direct absorption of photons by the compound. Indirect or sensitized photolysis is the result of energy transfer to the compound from some other molecule that has adsorbed radiation.

Direct Photolysis

In natural environments, the rate of light absorption at any wavelength λ, $R_{a\lambda}$ (photons/ℓ-s-nm), is directly proportional to the concentration of the absorbing compound, c(mole/ℓ).

$$R_a = K_{a\lambda} c \qquad (39)$$

where

$K_{a\lambda}$ = specific adsorption rate at wavelength λ (photons/mole-nm-s)

The specific absorption rate at any given wavelength is dependent on the rate at which light energy of that wavelength is incident on the compound [the scaler irradiance, $I_o(\lambda)$ (photons/cm^2-s-nm))], and the extent to which the compound absorbs light of that wavelength [the molar absorptivity, ε_λ(ℓ/mole-cm)]:

$$K_{a\lambda} = 1000\ \varepsilon_\lambda I_o(\lambda) \qquad (40)$$

In natural waters, UV-light of wavelength greater or equal to 295 nm and visible light up to 700 to 800 nm may contribute to photolysis. However, for the majority of compounds light absorption is most significant in the UV range (295-400 nm). The total specific adsorption rate, K_a, is determined by integrating $K_{a\lambda}$ over the wavelength spectrum of the incident light:

$$K_a = 1000 \int_\lambda \varepsilon_\lambda I_o(\lambda) d\lambda \qquad (41)$$

The total rate of light absorption is then the product of K_a and the molar concentration of the compound. If all the light absorbed were converted to photoreaction, the rate of decay due to photolysis would simply equal the rate of absorption:

$$\frac{dc}{dt} = -K_a c \qquad (42)$$

In fact, the absorption-reaction step has a low efficiency and equation (42) must be modified by the fraction of absorbed light that causes chemical change; the quantum yield, ϕ:

$$\frac{dc}{dt} = -\phi K_a c \qquad (43)$$

The quantum yield is an inherent property of the compound that may be readily computed from kinetic data obtained in the laboratory. It may be lowered by interactions of the compound with molecules called quenchers that remove the excess energy from the compound returning it from its electronically excited state to its ground state. Oxygen is the predominant quencher in natural water systems. The quantum yield may be increased by chemical reaction of the electronically excited compound with another molecule. It may also be altered by adsorption of the compound on suspended solids. In general, because of the short excited state lifetime (usually < 10 ns) and low concentrations of the pollutants of concern, natural photolysis and photolysis in pure air-saturated water are assumed equivalent (5).

Sensitized Photolysis

In addition to absorbing energy directly from photons, photoreactive compounds may take up energy from certain compounds called photosensitizers that have absorbed light. Photosensitizers are compounds capable of achieving a relatively long-lived electronically excited state called the triplet state. Humic materials are the most common sensitizers in natural waters.

The quantitative expression of sensitized photolysis includes the rate of light absorption by the sensitizer and quantum yields for the three steps involved in the photodegradation: (1) formation of the triplet state photosensitizer (ϕ_s), (2) transfer of energy to the photoreactive compound (ϕ_t)

and, (3) degradation of the electronically excited compound (ϕ). The resulting rate equation is:

$$\frac{dc}{dt} = -[\phi_s \phi_t \phi] K_{a_s} [s] \qquad (44)$$

where

s = concentration of sensitizer

K_{a_s} = total specific absorption rate of the sensitizer

The quantum yield defining the fraction of triplet energy transferred to the photoreactive compound, ϕ_t, is directly proportional to the concentration of the photoreactive compound:

$$\phi_t = K_t c \qquad (45)$$

If the quantum yields and the concentration of sensitizer are assumed constant, Eq. (44) reduces to a form identical to the rate expression for direct photolysis (Eq. 43):

$$\frac{dc}{dt} = -K'c \qquad (46)$$

where

$$K' = \phi_s \phi K_t [s]$$

Light Attenuation

Because the rates of direct and sensitized photolysis depend on the rate at which light energy of specific wavelengths is incident on the photoreactive compound, they vary with the time of day, the time of year, and the depth of the water body. Photolysis is maximum when the attenuation of sunlight in the atmosphere and in the water is minimum. Minimum attenuation in the atmosphere occurs when the pathlength through the atmosphere is a minimum, i.e. when the solar altitude is maximum. Thus, photolysis at the water surface is maximum at midday in summer. Light attenuation in the water is controlled by photoplankton and suspended solids concentrations that vary with flow and time of year. In general, photolysis is most significant in summer and least significant in winter.

Ultraviolet light intensity at the water surface is computed from recently published analytical expressions relating light attenuation to solar altitude, ozone and aerosol light absorption, and aerosol and air molecule light scattering (6,7). Following Zepp and Cline (8) surface intensity of visible light is computed using equations described by Leighton (9).

Light attenuation in water is a first-order process described by an equation of the form:

$$I(\lambda,z) = I(\lambda,o)e^{-Ke_{\lambda}z} \qquad (47)$$

where

Ke_{λ} = attenuation coefficient for light of wavelength λ (m^{-1})

z = depth (m)

Calculation Procedure

The model currently considers only direct photolysis. The calculation procedure follows Zepp and Cline (8). From a user specified location and season, atmospheric light intensities are computed. Using user specific light attenuation coefficients, the average light intensity in each water column segment of the model is then computed. Molar absorptivities of the chemical under study are combined with the segment light intensities to compute the rate of light absorption by the compound in accordance with equation (35). Given the quantum yield, photolysis rate constants are then computed. The average daily photolysis rate is determined by averaging computed rates for solar altitude increments up to the maximum solar altitude for the specified location and season.

3.2.3 Hydrolysis

Hydrolysis is a reaction in which a cleavage of a molecular bond of the compound and the formation of a new bond with the hydrogen and hydroxyl components of the water molecule results. Hydrolytic reactions are usually mediated by an acid or base and are identified in that fashion. To a more limited degree, there may also be a neutral reaction with water. By its nature, the rate of the reaction is a function of pH and, as with most chemical reactions, temperature.

It is a common phenomenon in many chemical and biochemical processes. In the biochemical processes, the fundamental food substances, such as carbohydrates, lipids and proteins are decomposed in this manner by various enzymes. These reactions are discussed under the Biodegradation Section which follows. In chemical processes, certain salts undergo hydrolysis. Salts formed in neutralization of a strong acid by a weak base or of a strong base by a weak acid yield acidic and alkaline reactions respectively, because of the higher concentrations of hydrogen or hydroxyl ion. The hydrolysis of organic chemicals, in some cases, is brought about by both biochemical as well as chemical factors and it is difficult to distinguish between them in prototype and certain laboratory conditions. It is pertinent to discuss each separately and to examine the factors which affect the individual processes.

The reaction equation, fundamentally second order, containing the product of the concentration of the chemical and either the acid, or alkaline concentration, in general, may be expressed as:

$$\frac{dc}{dt} = -Kc \qquad (48)$$

in which

$$K = K_a[H]^+ \text{ for acid hydrolysis}$$

$$= K_b[OH]^- \text{ for alkaline hydrolysis}$$

$$= K_n[H_2O] \text{ for neutral hydrolysis}$$

The effect of pH on the reaction may be quite pronounced. Due to the acid and base catalytic action, greater reaction coefficients are observed at the acid and alkaline pH extremes and minimum values in the neutral zone.

The effect of temperature is typical of chemical and biochemical reactions with the rate increasing with a rise in the temperature. The effect is usually expressed in terms of the Arrhenius equation, which relates the reaction coefficient to the activation energy (calories/mole), the absolute temperature and the gas constant. Based on this relation, the customary procedure of expressing the rate coefficient is as follows:

$$K = K_{20}\ \theta^{T-20} \qquad (49)$$

Reported laboratory and field (in soil experiments) indicate a range of θ of about 1.05-1.15 with an upper value of 1.2, i.e., temperature differences of between 5 and 15°C causing a doubling of the rate.

In addition to the effect of temperature and pH, there appear to be other factors which may influence the reaction rate, as is borne out by comparing rates of degradation in soil and in water. In general, the experimental data indicate the rate is greater in soil in some cases, by an order or more. This medium apparently catalyzes the degradation, perhaps due to the combined activity of both biological and chemical hydolysis.

The model considers acid, alkaline, and neutral hydrolysis. The user is required to input the rate constant for each and the pH in each segment of the model.

3.2.4 Biodegradation

Biodegradation encompasses the broad and complex processes of enzymatic attack by organisms on organic chemicals. Bacteria, and to a lesser extent fungi, are the mediators of biological degradation in natural systems. Dehalogenation, dealkylation, hydrolysis, oxidation, reduction, ring cleavage, and condensation reactions are all known to occur either metabolically or via co-metabolism. Co-metabolism refers to degradation of pesticides by microorganisms when the microbe is not capable of utilizing the pesticide as a substrate for growth. Sometimes the microbe does not even derive carbon or energy from the degradation, rather the pesticide is "caught up" in the overall metabolic reactions (10).

A chemical that is metabolized is used a a source of carbon, some other nutrient element or energy. When such compounds are introduced into a natural ecosystem the heterotrophs able to grow on them proliferate, the active population increasing in size with time.

In cometabolism the population density of the responsible species does not increase because it has no selective advantage in the presence of the compound and cannot use it as a nutrient. Because an increase in population density of species growing on a chemical is generally paralleled by an increase in degradation rate, cometabolism is characterized by the lack of an increase in disappearance rate with time after introduction of the chemical.

Metabolic reactions follow Monod or Michaelis-Mention enzyme kinetics. The degradation rate and bacterial growth rate can be expressed as:

$$\frac{dc}{dt} = - \frac{V_{max} c\ B}{k_M + c} \tag{50}$$

$$\frac{dB}{dt} = - a \frac{dc}{dt} \tag{51}$$

c = pesticide concentration

t = time

V_{max} = maximum rate of substrate utilization

B = bacteria concentration

k_M = Michaelis half saturation constant

a = yield coefficient for bacteria utilizing pesticide.

Values of k_M typically range from 0.1 to 10 mg/ℓ.

In general, chemical concentration is much less than the half-saturation constant and equation (50) reduces to:

$$\frac{dc}{dt} = - \frac{V_{max}}{K_M} cB = - K_b cB \tag{52}$$

This equation is used in the model to describe biodegradation and therefore the user is required to specify the rate constant, K_b, and for each segment, the bacterial concentration.

Specification of the proper biomass is critical since the degradation rate is directly proportional to it. Obviously, it is the concentration of bacteria capable of degrading the chemical under study that must be specified. However, for chemicals whose degradative pathway is a nonspecific enzymatic reaction such as hydrolysis use of total biomass may be sufficient.

3.2.5 Adsorption

As discussed in the development of the equations describing transport, sorption kinetics are not considered in the modeling framework. Instead, local equilibrium is assumed between the dissolved and particulate phases. This assumption implies that in comparison to any of the other processes occurring in the system, the sorption-desorption equilibrium is achieved so quickly that in describing the other processes the sorption-equilibrated concentrations can be found.

A linear isotherm relationship (equation (3)) is used to describe the equilibrium sorption. This type relationship has been observed in numerous adsorption studies (e.g., 11, 12, 13, 14) and is the most frequently used isotherm for describing organic chemical adsorption in soils and sediments (15, 16).

The partition coefficient describing the linear isotherm at a fixed solids concentration has been shown for numerous chemicals to depend on the concentration of adsorbing solids in the following fashion (17, 18):

$$\P = \frac{\beta}{m^{\alpha}} + \P_{\infty} \qquad (53)$$

where

m = concentration of solids
α, β = empirical constants
$\P_{\infty}$ = limiting partition coefficient at high solids concentration

For most chemicals $\P_{\infty}$ was found to be zero and is not considered in the 1.

The model uses this solids-dependent partitioning to compute the particulate and dissolved components of the chemical under study. A constant partitioning condition may be simulated by setting b equal to the partition coefficient and α to zero.

SECTION 4

STRUCTURE OF COMPUTER CODE

4.1 OVERVIEW

WASTOX was developed as a general purpose computer program for modeling the fate of toxic chemicals in any water body. It is based on the Water Analysis Simulation Program (WASP)(20) which was developed for modeling conventional pollutants in water bodies. The major differences between WASTOX and WASP are in the way transport is handled and in the reaction kinetics. In WASP flow and dispersion are assumed to be the same for all constituents being modeled. To account for the differences in flow and dispersion between dissolved chemical and adsorbed chemical and the multiple transport processes affecting each, WASTOX considers groups of flows and dispersions that are applied to either dissolved chemical or adsorbed chemical and solids, or both. In addition, the complete freedom allowed the user of WASP in specifying the reaction kinetics does not exist in WASTOX. Because WASTOX is directed to toxic chemicals only, the kinetics and associated input have been incorporated. The user may add to the kinetic processes but may not completely respecify them.

WASTOX consists of a mainline and twenty-eight subroutines. The mainline controls the assignment of logical units to the disk files used to store certain inputted information and the computational results and calls the subroutines. The subroutines may be separated by function into the categories input, computation, output, and utility. A list of the subroutines by category is given in Table 1.

TABLE 1. Subroutines comprising WASTOX

Mainline

RTWASP

Input	Computation	Output	Utility
WASP2	GREEN	WAS16	ABORT
WASP3	SPECIR	WSTSS3	SCALF
WAS3A	TSLAM		BWRITE
WASP4	WAS12		BREAD
WASP5	WAS12B		FILEOC
WASP6	WAS15		FILEOP
WASP7	WASP8		RESET
PHOTO	WASPB		
WASP9	WTXSS1		
WAS10	WTXSS2		
WAS11	WTXSS3		
	WTXSS4		

4.2 SUBROUTINES

WASP2

WASP2 initializes several variables and reads model identification information, the number of segments into which the water body is divided, the number of constituents being modeled, and system by-pass options. (Card Group A)

WASP3

WASP3 reads the input related to dispersion between segments. Depending on which of the six possible options is chosen, dispersions (E) and associated areas (A) and characteristic lengths (L) or exchanges (EA/L) are read in as constant values or variable in time as broken line approximations. (Card Group B)

WAS3A

WAS3A reads the volume of each segment either as a constant or as a timevariable function represented by a broken line approximation. (Card Group C)

WASP4

WASP4 reads the input related to flow between segments. Depending on which of three possible options is chosen, flows are read in as constants or as time-variable functions represented by broken line approximations. Flows are converted from their input units of cubic feet per second to million gallons per day. (Card Group D)

WASP5

WASP5 reads the concentrations of each constituent modeled at the boundaries of the model where a flow or dispersion (exchange) occurs. Depending on which of three possible options is chosen, boundary concentrations are read in as constants or as time-variable functions represented by broken line approximations. (Card Group E)

WASP6

WASP6 reads the mass rate of discharge into the water body of the constituents modeled (forcing functions). Depending on which of three possible options is chosen, forcing functions are read in as constants or as timevariable functions represented by broken line approximations. (Card Group F)

WASP7

WASP7 reads the parameters for each segment, the kinetic constants, and any miscellaneous time functions. The number of parameters and constants read in is computed internally for the current kinetic structure of subroutine WASPB. To add parameters and constants for any modifications of the kinetics requires changing the calculation of NPAM and NCONS. Note that for NPAM > 11 or NCONS > 30 the size of arrays PARAM and CONST in COMMON/MAIN/ must be changed. (Card Groups G,H and I)

PHOTO

PHOTO reads the coefficients necessary to compute the first-order photolysis rate constant and calls the subroutines GREEN, SPECIR, and TSLAM that compute the rate constant. The photolysis input and rate constant calculation may be bypassed using a switch. (Card Group J)

WASP9

WAS10 reads the print interval. (Card Group M)

WAS11

WAS11 reads the integration time step and the total time of the run. (Card Group N)

GREEN

GREEN computes the time of day for a given solar zenith angle, latitude, longitude, and ephemeride data. This information is used in subroutine SPECIR and TSLAM.

SPECIR

SPECIR computes the direct and diffuse UV spectral irradience at the water surface for use in calculating the photolysis rate constants.

TSLAM

TSLAM computes the direct and diffuse visible irradiance at the water surface for use in calculating the photolysis rate constants.

WAS12-WAS12B

WAS12 and WAS12B compute the transport component of the time derivative and add in any discharges or forcing functions.

WAS15

WAS15 performs the numerical integration using an Euler scheme. It also is the time counter for the model.

RESET

RESET recomputes the break times for time variable functions to repeat the function for times greater than the time of the last break in the function.

WTXSS1

steady-state solution subprogram which writes flow and bulk dispersion coefficients onto a disk file.

WTXSS2

accesses WASPB to determine reaction coefficients and then combines these with the transport coefficients to form steady-state solution subprogram which calculates each element of the coefficient matrix .

WTXSS3

sequentially computes the concentration vector for each system, and prints out steady-state concentration for each system.

WTXSS4

solves the set of simultaneous equations defined by the coefficient matrix and the concentration vector.

WASP8

WASP8 evaluates the slopes of the broken-line approximations used to represent time variable flows, dispersions, boundary conditions, and miscellaneous kinetic functions at each change in slope.

WASPB

WASPB computes the transfer and reaction components of the derivative. Rates of photolysis, hydrolysis, biodegradation and volatilization are computed. The fraction of chemical dissolved and adsorbed is computed from the sorption partition coefficient and the porosity and solids concentration of each segment. Segment concentrations are written to disk files at specified intervals.

WAS16

WAS16 reads the names, variable numbers and segment numbers for the variables to be printed. The times and concentrations are read from the disk files generated in WASPB during the simulation and printed.

ABORT

ABORT prints the reason for the termination of the run due to a user generated error.

SCALF

SCALF modifies the values in an array by a scale factor. The scaling operation may be a multiplication, division, addition or subtraction.,

BWRITE

BWRITE writes information for VAL and T onto a specified disk file beginning with a specified record.

BREAD

BREAD reads information into arrays VAL and T from a specified disk file beginning with a specified record.

DEC PDP Subroutines

Two special subroutines were written for the DEC computer system. These subroutines FILEOP and FILEOC were necessitated due to the way the DEC operating system handles disk output, i.e., requiring separate core buffers for each disk file. FILEOP and FILEOC permit the disk files to share a common disk buffer, reducing the excessive core requirements required for separate buffers, at little cost to execution time.

SECTION 5

PREPARATION OF DATA INPUT

5.1 INTRODUCTION

The computer code requires that all advective transport be specified as flows. The flows resulting from the settling and resuspension velocities in equation (22) are the product of the velocity and the interfacial area of the segments associated with the velocity. Flows are inputted in groups (fields) that are applied to dissolved chemical, or particulate chemical and solids, or both. Most models will have separate flow fields for the hydrodynamic flows, settling flows, resuspension flows, and bed sedimentation flows.

Dispersion coefficients are also inputted in groups or fields that are applied to dissolved chemical, or particulate chemical and solids, or both. Most models will have separate dispersion fields for water column dispersion and interstitial water diffusion.

The state variables in the model are termed systems. System 1 is total chemical and systems 2 through N are solids types. The maximum number of systems is 4 (i.e., a maximum of 3 solids types).

To properly account for certain kinetic processes the model must know which segments are water column segments. This is accomplished by requiring that in the segment numbering scheme chosen by the user the water column segments be numbered from 1 to the number of water column segments and the bed segments be numbered from one plus the number of water column segments to the total number of segments.

5.2 SUMMARY OF CARD GROUPS

Card Group

A. Model Identification and System Execution Options

1. Program Option
2. Model Identification Numbers
3. Title Card
4. Solution Type
5. System Execution Options

B. Exchange Coefficients

1. Input Option Number: Number of Exchange Fields
2. Number of Exchanges; Number of Systems Affected; Title
3. System Scale Factors
4. Exchange Coefficients

Card groups 2-4 are read for each exchange field

C. Segment Volumes

1. Number of Volumes; Input Option Number
2. Volumes

D. Flows

1. Input Option Number; Number of Flow Fields
2. Number of Flows: Number of Systems Affected; Title
3. System Scale Factors
4. Flows

Card groups 2-4 are read for each flow field

E. Boundary Conditions

1. Number of Boundary Conditions; Input Option Number
2. Boundary Conditions

Cards 1-2 are input for each system in the model

F. Forcing Functions

1. Number of Forcing Functions; Input Option Number
2. Forcing Functions

Cards 1-2 are inputted for each system in the model

SUMMARY OF CARD GROUPS (cont'd)

G. Parameters

1. Parameters

   Card group is inputted for each segment in the model

H. Constants

1. Constants

I. Miscellaneous Time Functions

1. Number of Time Functions
2. Function Name; Number of Breaks in Function

   Cards 2-3 are inputted for each time function in the model

J. Photolysis

1. Execution Switch
2. Number of Wavelengths
3. Toxicant Molar Extinction Coefficient
4. Toxicant Quantum Yield
5. Latitude; Longitude; Season
6. Extinction Coefficients
7. Cloud Cover Effect

K. Initial Conditions

1. Initial Conditions for each system in the model

L. Stability Criteria

1. Stability Criteria

M. Print Control

1. Print Interval

N. Integration Information

1. Integration Interval; Total Time

O. Display Parameters

1. Variable Names
2. Dump parameters

   Cards 1 and 2 are inputted for each system in the model

5.3 CARD GROUP A - MODEL IDENTIFICATION AND SYSTEM EXECUTION OPTIONS

The variables which appear on each card are as follows:

5.3.1 Exposure Concentration - Food Chain Option

5
PRGOPT

FORMAT(I5)

PRGOPT = 1; execute exposure concentration component of WASTOX only

PRGOPT = 2; execute food chain component of WASTOX only

PRGOPT = 3; execute exposure concentration and food chain components of WASTOX

5.3.2 Model Identification Numbers

5	10	15	20	25
MODEL	ISER	IRUN	NOSEG	NOSYS

FORMAT(5I5)

MODEL - model designation

ISER - series designation

IRUN - run number

NOSEG - number of model segments (maximum of 75)

NOSYS - number of systems (maximum of 4. Note that system 1 is toxicant and system 2 through N are solids types. Minimum number of systems is 2).

MODEL, ISER, IRUN, although not actually used by the program, can assist the user in maintaining a log of computer simulations.

5.3.3 Title

1	80
REAL TIME WASP - - - - - - - -	TOXICS MODEL

FORMAT(20A4)

Card columns 1-80 contain any information the user feels would be helpful in describing the run and identifying the output for later reference.

5.3.4 Time Variable or Steady State Solution

1
Type

FORMAT(A4)

Data input options:

TYPE - TIME VARIABLE; time variable solution requested

TYPE - STEADY STATE; steady state solution requested

Card columns 1 to 4 only are used to establish run type (e.g. TIME or STEA)

5.3.5 System Execution Options

1	2		
SYSEXC(1)	SYSEXC(2)	...	SYSEXC(NOSYS)

FORMAT(4I1)

SYSEXC(I) - 0, perform the kinetic and transport phenomena associated with system I (numerically integrate or iterate the differential equations).

1, bypass all kinetic and transport phenomena associated with system I (concentrations read as initial conditions for system I apply throughout simulation period).

5.4 CARD GROUP B - EXCHANGE COEFFICIENTS

Exchange coefficients may be inputted in one of two forms, actual exchange coefficients or, they may be calculated from inputted dispersion coefficients and accompanying crosssectional areas and characteristic lengths. Exchange coefficients for bed segments are assumed to be the product of porosity and the exchange coefficient.

5.4.1 Data Input Option Number; Number of Exchange Fields

```
    5   10
IROPT NRFLD
FORMAT(2I5)
```

Data input options:

IROPT - 1, constant exchange coefficients.

- 2, all exchange coefficients proportional to one piecewise linear approximation.
- 3, each exchange coefficient represented by its own piecewise linear approximation.
- 4, constant exchange coefficients calculated from the dispersion coefficient, cross-sectional area, and characteristic lengths specified for each interface.
- 5, all exchange coefficients proportional to one piece linear approximation, calculated from a piecewise linear dispersion coefficient approximation and respective cross-sectional areas, and characteristic lengths.
- 6, each exchange coefficient proportional to its own piecewise linear approximation, calculated from a piecewise linear approximation for the dispersion coefficients, cross-sectional area, and characteristic length specified for each area.

NRFLD - number of exchange fields.

If no exchange coefficients are to be read, set IROPT equal to zero, and continue with Card Group C.

Card types 2 through 4 are repeated NRFLD times, once for each separate exchange field incorporated in the model.

5.4.2 Number of exchanges, Number of systems affected, Exchange field title

5	10	21	80
NOR	NOSE		RTITL

FORMAT(2I5,10X,15A4)

NOR = number of exchange coefficients in this field

NOSE = number of systems that this exchange field is to be applied to

RTITL = any alphanumeric descriptor to describe this exchange field examples:

WATER COLUMN EXCHANGES
INTERSTITIAL WATER DIFFUSION

5.4.3 System Scale Factors

10	15	25		75
SCALES(1)	RSYS(1)	SCALES(2)	...	RSYS(NOSE)

FORMAT(4(E10.3,I5))

RSYS(I) = system affected by this exchange field

SCALES(I) = scale factor for system RSYS(I). All exchanges in this field are multiplied by SCALES(I) when the field is applied to system RSYS(I).

5.4.4 Exchange Coefficients

The data input format is determined by the option selected.

Option 1

Each card in this package contains the exchange coefficient information for four interfaces. The number of exchange coefficients read is equal to NOR. The last card is a scale factor for the exchange coefficients. The information on each card is described below:

10	15	20	30	35	40
BR(I)	IR(I)	JR(I)	BR(I+1)	IR(I+1)	JR(I+1)

50	55	60	70	75	80
BR(I+2)	IP(I+2)	JR(I+2)	BR(I+3)	IR(I+3)	JR(I+3)

FORMAT(4(F10.0,2I5))

BR(I) - exchange coefficient between segments IR(I) and JR(I) in million cubic feet per day.

IR(I),JR(I) - segments between which exchange takes place the order of the segments is not important; if a segment exchanges with a boundary, the boundary is specified as zero.

2	15	35
OP	FACTOR	UNITS

FORMAT(A2,3X,F10.2,2A10)

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value

UNITS - the units of the exchange coefficient after FACTOR has been applied.

NOTE: To request no scale factor put the value 1. after column 5 but before column 16 on the scale factor card. Also leave columns 1 to 5 blank.

Option 2

The card package consists of two sub-packages. Subpackage I contains the exchange coefficient data, while sub-package II contains a detailed specification of the piecewise linear approximation to which all exchange coefficients are proportional.

Sub-Package I - Exchange Coefficients

Each card in this sub-package contains the exchange coefficient information for four interfaces. The number of exchange coefficients read is equal to NOR. The last card of this subpackage contains the scale factor for the exchange coefficients. The information on each card is described below:

10	15	20	30	35	40
BR(I)	IR(I)	JR(I)	BR(I+1)	IR(I+1)	JR(I+1)

50	55	60	70	75	80
BR(I+2)	IR(I+2)	JR(I+2)	BR(I+3)	IR(I+3)	JR(I+3)

FORMAT(4(F10.0,2I5))

BR(I) - ratio of the exchange coefficient between segments IR(I) and JR(I) to the piecewise linear approximation.

IR(I),JR(I) - segments between which exchange takes place

NOTE: the order of the segments is not important; if a segment exchanges with a boundary, the boundary is specified as zero.

2	15	35
OP	FACTOR	UNITS

FORMAT(A2,3X,F10.2,2A10)

OP - the operation (* / + or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of the exchange coefficient after FACTOR has been applied.

Sub-Package II - Piecewise Linear Approximation

The number of breaks required to describe the broken line approximation is followed by a time series describing the broken line approximation. Each time series element consists of two parts; an exchange value and a time (normal time scale is days). The last card of this subpackage contains the scale factor for exchange value. The input is as follows:

5
NOBRK

FORMAT(I5)

NOBRK - number of values and times used to describe the piecewise linear approximation.

10	20	30	40	50	60	70	80
RT(I)	T(I)	RT(I+1)	T(I+1)	RT(I+2)	(T+2)	RT(I+3)	T(I+3)

FORMAT(8F10.0)

RT(I) - value of the approximation at time T(I), in million cubic feet per day.

T(I) - time in days; if the length of the simulation exceeds T(NOBRK), the piecewise linear approximation will repeat itself, starting at time T(1); i.e., the approximation is assumed to be periodic with period equal to T(NOBRK), this holds true for all piecewise linear functions of time.

2	15	35
OP	FACTOR	UNITS

FORMAT(A2,3X,F10.2,2A10)

OP - the operation (* / + - or **) of the scale factor

FACTOR - the scaling value

UNITS - the units of the exchange value after FACTOR has been applied.

Option 3

Each exchange coefficient is defined by a package of cards consisting of two sub-packages. The first sub-package identifies the two segments between which the exchange will take place, and the number of values comprising the piecewise linear approximation. The second subpackage defines the piecewise linear approximation which describes the exchange coefficient and a scale factor. The input is as follows:

SubPackage 1

5	10	15
IR(I)	JR(I)	NOBRK(5)

FORMAT(2I3,I4)

IR(I),JR(I)	-	segments between which exchange takes place; NOTE: for exchange only, order of segments is not important. If segment exchanges with a boundary, the boundary is specified as zero.
NOBRK	-	number of values and times used to describe the piecewise linear approximation. All exchanges must have the same number of breaks.

SubPackage II - Piecewise Linear Approximation

This consists of a time series describing the piecewise linear approximation. Each time series element consists of two parts; an exchange value, and a time (normal time units days). The last card is a scale factor for the exchange value. The input is as follows:

RT(I)	T(I)	RT(I+1)	T(I+1)	RT(I+2)	T(I+2)	RT(I+3)	T(I+3)

FORMAT(8F10.0)

RT(I) - value of the piecewise linear approximation at time T(I) in million cubic feet per day.

T(I) - time in days. All break times must agree for all segments, i.e., T(1) must be the same for all exchanges, T(2) must be the same for all exchanges, etc.

2	15	35	40
OP	FACTOR	UNITS	IFLG

FORMAT(A2,3X,F10.2,2A10,I5)

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of the exchange value after FACTOR has been applied.

IFLG - flag set equal to 1, if this scale factor is to apply to all the remaining exchange coefficients in this field.
If IFLG = 1, then scale factor cards are not included for the remaining exchange coefficients in this field.

Option 4

Each card in this package contains the information to calculate the exchange coefficient for two interfaces. The number of dispersion coefficients is equal to NOR. The last card is a scale factor for the dispersion coefficient. The information on each card is described below:

10	20	25	30	35	40
E(I)	A(I)	IL(I)	JL(I)	IR(I)	JR(I)

50	60	65	70	75	80
E(I+1)	A(I+1)	IL(I+1)	JL(I+1)	IR(I+1)	JR(I+1)

FORMAT(2(2F10.0,2F5.0,2I5))

E(I) - dispersion coefficient for the interface between segment IR(I) and JR(I) in square miles per day.

A(I) - the interfacial crosssectional area between segments IR(I) and JR(I), in square feet.

IL(I) - the length of segment IR(I), with respect to the IR(I)-JR(I) interface, in feet.

JL(I) - the length of segment JR(I) in relation to the IR(I)-JR(I) interface, in feet. If a segment exchanges with a boundary, the characteristic length of the boundary should be set equal to the length of the segment with which it is exchanging.

IR(I),JR(I) - segments between which exchange takes place;

NOTE: for exchange only, order is not important--if a segment exchange with a boundary, the boundary is specified as zero.

2	15	35
OP	FACTOR	UNITS

FORMAT(A2,3X,F10.2,2A10)

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of the dispersion coefficient after FACTOR has been applied.

Option 5

The card package consists of two sub-packages. Sub-Package I contains the information necessary to calculate the exchange coefficients, while sub-package II contains a detailed specification of the piecewise linear approximation to which the dispersion coefficients contained in sub-package I are proportional.

Sub-Package I

Each card in this sub-package contains the information necessary to calculate the exchange coefficients for two interfaces. The number of dispersion coefficients is equal to NOR. The last card is a scale factor for the dispersion coefficient. The information on each card is described below:

10	20	25	30	35	40
E(I)	A(I)	IL(I)	JL(I)	IR(I)	JR(I)

50	60	65	70	75	80
E(I+1)	A(I+1)	IL(I+1)	JL(I+1)	IR(I+1)	JR(I+1)

FORMAT(2(2F10.0,2F5.0,2I5))

E(I) - the ratio of the dispersion coefficient between segment IR(I) and JR(I) to the piecewise linear approximation.

A(I) - the interfacial crosssectional area between segments IR(I) and JR(I), in square feet.

IL(I) - the length of segment IR(I) in relation to the IR(I)-JR(I) interface, in feet.

JL(I) - the length of segment JR(K) in relation to the IR(I)-JR(I) interface, in feet. If a segment exchanges with a boundary, the characteristic length of the boundary should be set equal to the length of the segment with which it is exchanging.

IR(I),JR(I) - segments between which exchange takes place;

NOTE: for exchange only, order is not important.

2	15	35
OP	FACTOR	UNITS

FORMAT(A2,3X,F10.2,2A10)

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of the dispersion coefficient after FACTOR has been applied.

Sub-Package II - Piecewise Linear Approximation

The number of breaks required to describe the piecewise linear approximation is followed by a time series describing the piecewise linear approximation. Each time series element consists of two parts; a dispersion coefficient and a time (normal units are days). The last card is the scale factor for the dispersion coefficient. The input is as follows:

5
NOBRK

FORMAT(I5)

NOBRK - number of values and times used to describe the piecewise linear approximation.

10	20	30	40	50	60	70	80
RT(I)	T(I)	RT(I+1)	T(I+1)	RT(I+2)	T(I+2)	RT(I+3)	T(I+3)

FORMAT(8F10.0)

RT(I) - value of the piecewise linear approximation at time T(I), in square miles per day.

T(I) - time in days.

2	15	35
OP	FACTOR	UNITS

FORMAT(A2,3X,F10.2,2A10)

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of the dispersion coefficient after FACTOR has been applied.

Option 6

Each exchange coefficient is defined by a package of cards consisting of three sub-packages. The first sub-package defines the interfacial cross-sectional area and the characteristic length. The second sub-package identifies the two segments between which the exchange will take place, and defines the number of values comprising the piecewise linear approximation. The third sub-package defines the piecewise linear approximation which describes the dispersion coefficient.

Sub-Package I

The sub-package defines the interfacial cross-sectional area and the characteristic length of the segments involved, also the scale factors.

```
    10        20
 A(I)    A(I+1). . .A(NOR1)    A(NOR)
 FORMAT(8F10.0)
```

A(I) - the interfacial cross-sectional area between segments in square feet.

```
  2      15       35
 OP   FACTOR   UNITS
```

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of the area after FACTOR has been applied.

```
     10        20
 XL(I)    XL(I+1) . . . XL(NOSEG-1)XL(NOSEG)
 FORMAT(8F10.0)
```

XL(I) - the length of the segment in the direction of the dispersion, in feet. If a segment exchanges with a boundary, the characteristic length of the boundary should be set equal to the length of the segment with which it is exchanging.

2	15	35
OP	FACTOR	UNITS

FORMAT(A2,3X,F10.2,2A10)

OP - the operation (* / + - or **) of the scale factor)

FACTOR - the scaling value

UNITS - the units of the characteristic length after FACTOR has been applied.

Sub-Package II

5	10	15
IR(I)	JR(I)	NOBRK

FORMAT(2I3,I4)

IR(I),JR(I) - segments between which exchange takes place;
NOTE: for exchange only, order is not important

NOBRK - number of values and times used to describe the piecewise linear approximation. All exchanges must have the same number of breaks.

Sub-Package III - Piecewise Linear Approximation

This consists of a time series describing the piecewise linear approximation. Each time series element consists of two parts; a dispersion coefficient, and a time (consistent with the normal time scale of the model). The last card is a scale factor for the dispersion coefficient. The input is as follows:

10	20	30	40	50	60	70	80
RT(I)	T(I)	RT(I+1)	T(I+1)	RT(I+2)	T(I+2)	RT(I+3)	T(I+3)

FORMAT(8F10.0)

RT(I) - value of the piecewise linear approximation at time T(I), in square miles per day.

T(I) - time in days; all break times must agree for all segments, i.e., T(1) must be the same for all exchanges, T(2) must be the same for all exchanges, etc.

```
 2          15          35
OP      FACTOR       UNITS
FORMAT(A2,3X,F10.2,2A10)
```

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of the dispersion coefficient after FACTOR has been applied.

IFLG - flag set equal to 1 if this scale factor is to apply to all the remaining exchange coefficients in this field.
If IFLG = 1, then scale factor cards are not included for the remaining exchange coefficients in this field.

5.5 CARD GROUP C - VOLUMES

5.5.1 Data Input Option Number; Number of Volumes

5	10
IVOPT	NOV

FORMAT(2I5)

Data input options:

IVOPT - 1, constant volumes

2, all volumes proportional to one piecewise linear approximation.

3, each volume is represented by its own piecewise linear approximation.

NOV - number of volumes; normally NOV is equal to NOSEG, the number of segments;

5.5.2 Volumes

The data input format is determined by the option selected.

Option 1

Each card in this package contains the volume information for eight segments. The number of volumes is equal to NOV. The last card is the scale factor for the volumes. The information on each card is described below:

10	20	30		70	80
BVOL(I)	BVOL(I+1)	BVOL(I+2)	. . . .	BVOL(I+6)	BVOL(I+7)

FORMAT(8F10.0)

BVOL(I) - volumes of segment I, in million cubic feet. The volumes are listed consecutively starting with segment 1, and ending with segment NOV.

```
2        15       35
OP      FACTOR    UNITS
FORMAT(A2,3X,F10.2,2A10)
```

OP - the operation (* / + - or **) of the scale factor

FACTOR - the scaling value

UNITS - the units of the volume after FACTOR has been applied.

Option 2

The card package consists of two sub-packages. Sub-package I contains the volume data while sub-package II contains a detailed specification of the piecewise linear approximation to which all volumes are proportional.

Sub-Package I - Volumes

Each card in this subpackage specifies the volume ratios of eight segments. The number of volumes is equal to NOV. The last card is the scale factor for the volume ratios. The input is described below:

```
       10        20        30                80
BVOL(I)BVOL(I+1)BVOL(I+2) . . . BVOL(I+7)
FORMAT(8F10.0)
```

BVOL(I) - ratio of the volume in segment I to the piecewise line approximation. The ratios are listed consecutively, starting with segment 1 and ending with segment NOV.

```
OP      FORMAT    UNITS
FORMAT(A2,3X,F10.2,2A10)
```

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of the volume ratios after FACTOR has been applied.

Option 3

This package reads a separate piecewise linear volume function for each segment, from 1 through NOV. The last card is a scale factor for the volumes.

5
NOBRK

FORMAT(I5)

NOBRK - number of values and times used to describe the piecewise linear approximation. NOBRK must be the same for each broken line approximation.

10	20	30	40	50	60	70	80
VT(I)	T(I)	VT(I+1)	T(I+1)	VT(I+2)	T(I+2)	VT(I+3)	T(I+3)

FORMAT(8F10.0)

VT(I) - value of the piecewise linear approximation at time T(I), for segment I in million cubic feet.

T(I) - time in days; if the length of the simulation exceeds T(NOBRK), the approximation will repeat itself starting at time T(1), i.e., the approximation is assumed to be periodic with period T(NOBRK). All break times must agree for all segments, i.e., T(1) must be the same for all volumes, T(2) must be the same for all volumes, etc.

2	15	35	40
OP	FACTOR	UNITS	IFLG

FORMAT(A2,3X,F10.2,2A10,15)

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value. UNITS the units of the volumes after FACTOR has been applied.

IFLG - flag set equal to 1 if this scale factor is to apply to all the remaining volumes. If IFLG = 1 then scale factor cards are not included for the remaining volumes.

5.6 CARD GROUP D - FLOWS

5.6.1 Data Input Option Number; Number of Flow Fields

5	10
IQOPT	NOQF

FORMAT(2I5)

Data Input Options:

IQOPT - 1, constant flows.

2, all flows proportional to one piecewise linear approximation.

3, each flow is represented by its own piecewise linear approximation.

NOQF - number of flow fields.

If no flows are to be inputted, set IQOPT to zero and go to Card Group E. The maximum number of flow fields is 9.

Card types 2 through 4 are repeated NOQF times, once for each separate flow field incorporated in the model.

5.6.2 Number of flows, Number of systems affected, Flow direction switch, Flow field title

5	10	15	21	80
NOQ	NOSE	IDIRSW		QTITL

FORMAT(3I5,5X,15A4)

NOQ = number of flows in this field

NOSE = number of systems that this flow field is to be applied to

IDIRSW = switch that when set equal to 1 reverses the direction of all the flows in this field

QTITL = any alphanumeric descriptor to describe this flow field examples:

HYDRODYNAMIC FLOW
SETTLING OF SOLIDS
RESUSPENSION OF SOLIDS

5.6.3 System Scale Factors

10	15	25		75
SCALES(I)	QSYS(I)	SCALES(2)	. . .	QSYS(NOSE)

FORMAT(5(E10.3,I5))

QSYS(I) = system affected by this flow field

SCALES(I) = scale factor for system QSYS(I). All flows in this field are multiplied by SCALES(I) when the field is applied to system QSYS(I).

5.6.4 Flows

The data input format is determined by the option selected.

Option 1

Each card in this package contains the flow information for four interfaces, the number of flow specifications is equal to NOQ. The last card is a scale factor for the flows. The information on each card is described below:

10	15	20	30	35	40
BQ(I)	IQ(I)	JQ(I)	BQ(I+1)	IQ(I+1)	JQ(I+1)

50	55	60	70	75	80
BQ(I+2)	IQ(I+2)	JQ(I+2)	BQ(I+3)	IQ(I+3)	JQ(I+3)

FORMAT(4(F10.0,2I5)

BQ(I) - flow between segment IQ(I) and JQ(I) in cfs. Convention: if the flow value is positive, then flow is from segment JQ(I) to IQ(I).

IQ(I) - downstream segment

JQ(I) - upstream segment

If flow is from a segment to a boundary, then IQ(I) is set equal to zero; if a flow is from a boundary to a segment, then JQ(I) is set equal to zero.

2	15	35
OP	FACTOR	UNITS

FORMAT(A2,3X,F10.2,2A10)

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of the flows after FACTOR has been applied.

Option 2

The card package consists of two sub-packages. Sub-package I contains the flow routing while sub-package II contains a detailed specification of the piecewise linear approximation to which all the flows are proportional.

Sub-Package I - Flows

Each card in this sub-package contains the flow information for four interfaces. The number of flow specifications is equal to NOQ. The last card is a scale factor for the flows. The information on each card is described below:

10	15	20	30	35	40
BQ(I)	IQ(I)	JQ(I)	BQ(I+1)	IQ(I+1)	JQ(I+1)

50	55	60	70	75	80
BQ(I+2)	IQ(I+2)	JQ(I+2)	BQ(I+3)	IQ(I+3)	JQ(I+3)

FORMAT(4(F10.0,2I5)

BQ(I) - ratio of the flow between segments IQ(I) and JQ(I) to the piecewise linear flow approximation.

IQ(I) - downstream segment

JQ(I) - upstream segment

If flow is from a segment to a boundary, then IQ(I) is set equal to zero, if a flow is from a boundary to a segment, then JQ(I) is set equal to zero.

2	15	35
OP	FACTOR	UNITS

FORMAT(A2,3X,F102,2A10)

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of the flow ratios after FACTOR has been applied.

Sub-Package II - Piecewise Linear Flow

The number of breaks required to describe the piecewise linear approximation is followed by a time series describing the piecewise linear flow approximation. Each time series element consists of two parts; a flow and a time. The last card is a scale factor for the flows. The input is as follows:

5
NOBRK

FORMAT(I5)

NOBRK - number of values and times used to describe the piecewise linear approximation.

10	20	30	40	50	60	70	80
QT(I)	T(I)	QT(I+1)	T(I+1)	QT(I+2)	T(I+2)	QT(I+3)	T(I+3)

FORMAT(8F10.0)

QT(I) - value of the piecewise linear approximation at time T(I), in cubic feet per second.

T(I) - time in days, if length of the simulation exceeds T(NOBRK), the broken line function will repeat itself, starting at time T(I), i.e., the approximation is assumed to be periodic, with period equal to T(NOBRK).

2	15	35
OP	FACTOR	UNITS

FORMAT(A2,3X,F10.2,2A10)

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of the flow after FACTOR has been applied.

Option 3

Each flow is defined by a package of cards consisting of two sub-packages. The first subpackage identifies the two segments between which the flow occurs, and the number of values comprising the piecewise linear flow approximation. The second subpackage defines the piecewise linear approximation which describes the flow. The input is as follows:

SubPackage I

5	10	15
IQ(I)	JQ(I)	NOBRK

FORMAT(3I5)

IQ(I) - downstream segment, flow from segment JQ(I) to IQ(I), assuming positive flow.

JQ(I) - upstream segment flow from segment IQ(I), assuming positive flow.

NOBRK - number of values and times used to describe the broken line approximation. All flows must have the same number of breaks.

SubPackage II

Sub-package II is a time series describing the piecewise linear approximation. Each time series element consists of two parts; a flow and a time. The last card is a scale factor for the flows. The input is as follows:

10	20	30	40	50	60	70	80
QT(I)	T(I)	QT(I+1)	T(I+1)	QT(I+2)	T(I+2)	QT(I+3)	T(I+3)

FORMAT(8F10.0)

QT(I) - value of the piecewise linear flow approximation at time T(I) in cfs.

T(I) - time in days, if the length of the simulation exceeds T(NOBRK) the broken line function will repeat ifself, starting at time T(1). All break times must agree for all segments; i.e., T(1) must be the same for all flows, T(2) must be the same for flows, etc.

2	15	35
OP	FACTOR	UNITS

FORMAT(A2,3X,F10.2,2A10)

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of the flow after FACTOR has been applied.

IFLG - flag set equal to 1 if this scale factor is to apply to all the remaining flows in this field.
If IFLG = 1 then scale factor cards are not included for the remaining flows in this field.

5.7 CARD GROUP E - BOUNDARY CONDITIONS

All input is read NOSYS times; once for each system of the model.

5.7.1 Data Input Option Number; Number of Boundary Conditions

5	10
IBCOP(I)	NOBC(I)

FORMAT(2I5)

Data Input Options:

IBCOP(I) - 1, constant boundary conditions
2, all boundary conditions proportioned to one piecewise linear approximation.
3, each boundary condition represented by its own piecewise linear approximation.

NOBC(I) - number of boundary conditions used for system I.

If no boundary conditions are to be inputted, set NOBC(I) equal to zero, and continue with the next system, or go to the next card group.

5.7.2 Boundary Conditions

The data input format is determined by the option selected.

Option 1

10	15	25	30	40
BBC(I)	IBC(I)	BBC(I+1)	IBC(I+1)	BBC(I+2)

45	55	60	70	75
IBC(I+2)	BBC(I+3)	IBC(I+3)	BBC(I+4)	IBC(I+4)

FORMAT(5(F10.0,I5))

BBC(I) - boundary condition of segment IBC(I) in mg/ℓ.

IBC(I) - segment number to which boundary condition BBC(I) is to be applied.

2	15	35
OP	FACTOR	UNITS

FORMAT(A2,3X,F10.2,2A10)

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of the boundary condition after FACTOR has been applied.

Option 2

This card package consists of two sub-packages. Sub-package I contains boundary condition data, while sub-package II contains a detailed specification of the piecewise linear approximation to which all boundary conditions are to be proportional.

Sub-Package I

Each card in this sub-package contains the boundary condition information for five segments. The number of boundary condition specifications is equal to NOBC. The last card of the package is the scalefactor for the boundary conditions. The information on each card is described below:

10	15	25	30	40
BBC(I)	IBC(I)	BBC(I+1)	IBC(I+1)	BBC(I+2)

45	55	60	70	75
IBC(I+2)	BBC(I+3)	IBC(I+3)	BBC(I+4)	IBC(I+4)

FORMAT(5(F10.0,I5))

BBC(I) - ratio of the boundary condition for segment IBC(I) to the piecewise linear approximation.

IBC(I) - segment number.

2	15	35
OP	FACTOR	UNITS

FORMAT(A2,3X,F10.2,2A10)

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of boundary condition specifications after FACTOR has been applied.

Sub-Package II - Piecewise Linear Boundary Condition Approximation

The number of breaks required to describe the piecewise linear boundary condition approximation is followed by a time series describing the boundary approximation. Each time series element consists of two parts; boundary concentration, and a time. The last card is a scale factor. The input is as follows:

5
NOBRK
FORMAT(I5)

NOBRK - number of values and times used to describe the piecewise linear approximation.

10	20	30	40	50	60	70	80
BCT(I)	T(I)	BCT(I+1)	T(I+1)	BCT(I+2)	T(I+2)	BCT(I+3)	T(I+3)
FORMAT(8F10.0)							

BCT(I) - value of the broken line approximation at time T(I) mg/ℓ.

T(I) - time at breaks in broken line approximation in days.

If the length of the simulation exceeds T(NOBRK), the piecewise linear approximation is repeated, starting at T(1), i.e., the approximation is assumed to have period equal to T(NOBRK).

2	15	35
OP	FACTOR	UNITS
FORMAT(A2,3X,F10.2,2A10)		

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling values.

UNITS - the units of the boundary concentration after FACTOR has been applied.

Option 3

Each boundary condition is defined by a package of cards consisting of two sub-packages. The first sub-package identifies the segment associated with the boundary condition and the number of values comprising the piecewise linear approximation. The second sub-package defines the piecewise linear approximation which describes the boundary conditions. All boundary condisions for one system must have the same number of breaks. The input is as follows:

SubPackage I

5	10
IBC(I)	NOBRK

FORMAT(2I5)

IBC(I) - boundary segment number.

NOBRK - number of values and times used to describe the broken line approximation. The number of breaks must be equal for all boundary conditions within a system.

Sub-Package II - Piecewise Linear Boundary Condition Approximation

The segment number and the number of breaks required to describe the broken line approximation is followed by a time series describing the broken line approximation. Each time series element consists of two parts: a boundary concentration, and a time (consistent with the normal time scale of the model). The number of breaks must be the same for all boundary approximations. The last card is a scale factor for the boundary concentrations. The input is as follows:

10	15	25	30	40	45	70	75
BCT(I)	T(I)	BCT(I+1)	T(I+1)	BCT(I+2)	T(I+2)	BCT(I+4)	T(I+4)

FORMAT 5(F10.0,F5.0)

BCT(I) - value of the boundary approximation at time T(I) in mg/ℓ.

T(I) - time in days; if the length of the simulation exceeds T(NOBRK), the broken line approximation is repeated, starting at T(1), i.e., the approximation is assumed to be periidic, with period equal to T(NOBRK). All break times must agree for all segments, i.e., T(1) must be the same for all exchanges, T(2) must be the same for all exchanges, etc.

2	15	35	40
OP	FACTOR	UNITS	IFLG

FORMAT(A2,3X,F10.2,2A10,I5)

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of the boundary concentration after FACTOR has been applied.

IFLG - flag set equal to 1 if this scale factor is to apply to all the remaining boundary conditions.

If IFLG = 1 then scale factor cards are not included for the remaining boundary conditions.

5.8 CARD GROUP F - FORCING FUNCTIONS

All input is read NOSYS times, once for each system of the model.

5.8.1 Data Input Option Number; Number of Forcing Functions

5	10
IWOP(I)	NOWK(I)
FORMAT(2I5)	

Data Input Options:

IWOP(I) - 1, constant forcing functions

- 2, all forcing functions are proportioned to one piecewise linear approximation.

- 3, each forcing function represented by its own piecewise linear approximation.

NOWK(I) - number of forcing functions used for system I. NOTE: forcing functions may also be considered as sources (loads) or sinks of a water quality constitutent. If no forcing functions are to be inputted, set NOWK(I) to zero, and continue with next system or go to next card group if this is the last system.

5.8.2 Forcing Functions

The data input format is determined by the option selected.

Option 1

10	15	25	30	40
BWK(I)	IWK(I)	BWK(I+1)	IWK(I+1)	BWK(I+2)

45	55	60	70	75
IWK(I+2)	BWK(I+3)	IWK(I+3)	BWK(I+4)	IWK(I+4)

FORMAT(5(F10.0,I5))

BWK(I) - forcing function of segment IWK(I), in pounds per day.

IWK(I) - segment number to which forcing function BWK(I) is to be applied.

2	15	35
OP	FACTOR	UNITS

FORMAT(A2,3X,F10.2,2A10)

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of the forcing function after FACTOR has been applied.

Option 2

The card package consists of two sub-packages. Sub-package I contains the forcing function data, while sub-package II contains a detailed specification of the piecewise linear approximation to which all forcing functions are proportional.

Sub-Package I

Each card in this sub-package contains the forcing function information for five segments. The number of specifications is equal to NOWK(I). The last card is a scale factor for the forcing function information. The information on each card is described below:

10	15	25	30	40
BWK(I)	IWK(I)	BWK(I+1)	IWK(I+1)	BWK(I+2)

45	55	60	70	75
IWK(I+2)	BWK(I+3)	IWK(I+3)	BWK(I+4)	IWK(I+4)

FORMAT(5(F10.0,I5))

BWK(I) - ratio of the forcing function for segment IWK(I) to the piecewise linear approximation

IWK(I) - segment number to which forcing function BWK(I) is to be applied.

2	15	35
OP	FACTOR	UNITS

FORMAT(A2,3X,F10.2,2A10)

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of the forcing function ratio after FACTOR has been applied.

Sub-Package II - Piecewise Linear Forcing Function Approximation

The number of breaks required to describe the piecewise linear forcing function approximation is followed by a time series describing the forcing function. Each time series element consists of two parts; a function value and a time. The last card is the scale factor for the function value. The input is as follows:

5
NOBRK

FORMAT(I5)

NOBRK - number of values and times used to describe the piecewise linear approximation.

10	20	30	40	50	60	70	80
WKT(I)	T(I)	WKT(I+1)	T(I+1)	WKT(I+2)	T(I+2)	WKT(I+3)	T(I+3)

FORMAT(8F10.0)

WKT(I) - value of the forcing function at time T(I), in pounds per day.

T(I) - time in days; if the length of the simulation exceeds T(NOBRK), the forcing function approximation is repeated, starting at T(1), i.e., the approximation is assumed to be periodic, with period equal to T(NOBRK).

2	15	35
OP	FACTOR	UNITS

FORMAT(A2,3X,F10.2,2A10)

OP - the operation (* / + - or **) of the scale factor

FACTOR - the scaling value.

UNITS - the units of the forcing function after FACTOR has been applied.

Option 3

Each forcing function is defined by a package of cards consisting of two sub-packages. The first sub-package identifies the segment associated with the forcing function and the number of values comprising the piecewise linear approximation. The second sub-package defines the approximation which describes the forcing function. The input is as follows:

SubPackage I

5	10
IWK(I)	NOBRK

FORMAT(2I5)

IWK(I) - segment number which has forcing function BWK(I)

NOBRK - number of breaks used to describe the forcing function approximation. The number of breaks must be equal for all forcing functions within a system.

Sub-Package II - Piecewise Linear Forcing Function Approximation

The segment number and the number of breaks required to describe the piecewise linear forcing function approximation is followed by a time series, describing the forcing function. Each time series element consists of two parts: a function value and a time. The last card is scale factor for the forcing function. The input is as follows:

10	20	30	40	50	60	70	80
WKT(I)	T(I)	WKT(I+1)	T(I+1)	WKT(I+2)	T(I+2)	WKT(I+3)	T(I+3)

FORMAT(5(F10.0,F5.0))

WKT(I) - value of the forcing function at time T(I), in pounds per day.

T(I) - time in days; if length of the simulation exceeds T(NOBRK), the approximation is assumed to be periodic with period equal to T(NOBRK). All break times must agree for all segments; i.e., T(1) must be the same for all forcing functions, T(2) must be the same for all forcing functions, etc.

2	15	35	40
OP	FACTOR	UNITS	IFLG

FORMAT(A2,3X,F10.2,2A10,I5)

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value.

UNITS - the units of the forcing function after FACTOR has been applied.

IFLG - flag set equal to 1 if the scale factor is to apply to all the remaining forcing functions.
If IFLG = 1 then scale factor cards are not included for the remaining forcing functions.

5.9 CARD GROUP G - PARAMETERS

All input is read NOSEG times, once for each segment.

The definition of the parameters is set in the kinetics subroutine (WASPB). The number of parameters used in the model is dependent on the number of solids types considered.

5.9.1 Segment Parameters

5	15	20	30
ANAME(I)	PARAM(ISEG,I)	ANAME(I+1)	PARAM(ISEG,I+1)

35	45
ANAME(I+2)	PARAM(ISEG,I+2)...

FORMAT(5(1X,A4,F10.0))

ANAME(I) - a one to four alphanumeric character descriptive name for parameter PARAM(ISEG,I)

PARAM(ISEG,I) - the value of parameter ANAME(I) in segment ISEG.

Required Parameters

Parameter	Fortran Variable Name	Suggested ANAME	Description	Units
1	DEPTH	DPTH	Segment depth	meters
2	TDEPTH	TDPT	Depth of segment surface	meters
3	DWNSEG	DSEG	Segment downstream of current segment	
4	AREA	AREA	Area between current segment and downstream segment	ft^2
5	PH	PH	pH of segment	
6	TEMP	TEMP	temperature of segment	°C
7	WVEL	WVEL	Wind velocity 10 meters above the water surface at the location of the current segment	m/s

Required Parameters (cont'd)

Parameter	Fortran Variable Name	Suggested ANAME	Description	Units
8	BACW	BACW	concentration of compound degrading bacteria in water	num/ℓ (or units compatible with degradation rate constant)
9	BACS1	BCS1	concentration of compound degrading bac teria on solids type 1	num/mg (or units compatible with degradation rate constant)

IF ADDITIONAL SOLIDS TYPES ARE INCLUDED IN THE MODEL:

for each additional solids type add a parameter analogous to parameter 9. For example, if 3 solids types are considered (NOSYS=4) then a 10th and 11th parameter, BACS2 and BACS3, respectively, must be included.

5.10 CARD GROUP H - CONSTANTS

The definition of the constants is set in the kinetics subroutine (WASPB). The number of constants used in the model is dependent on the number of solids types considered.

5.10.1 Constants

5	15	20	30	35
ANAME(I)	CONST(I)	ANAME(I+1)	CONST(I+1)	ANAME(I+2)

45	50	60	65	75
CONST(I+2)	ANAME(I+3)	CONST(I+3)	ANAME(I+4)	CONST(I+4)

FORMAT(5(1X,A4,F10.0))

ANAME(I) - a one to four alpha-numeric character descriptive name for constant CONST(I).

CONST(I) - the value of constant ANAME(I).

Required Constants

Constant	Fortran Variable Name	Suggested ANAME	Description	Units
1	KD20	KD20	2nd Order biodegradation rate constant for dissolved toxicant at 20°C	ℓ/d-num (or units compatible with bacterial concentration BACW)
2	KDT	KDT	Temperature correction factor for biodegradation of dissolved toxicant	
3	KP20	KP20	2nd Order biodegradation rate constant for sorbed toxicant at 20°C	ℓ/dnum (or units compatible with bacterial concentration BACS)
4	KPT	KPT	Temperature correction factor for biodegradation of sorbed toxicant	
5	KHOH20	KHOH	2nd Order alkaline hydrolysis rate constant at 20°C	ℓ/mole-d
6	KHN20	KHN	1st Order neutral hydrolysis rate constant at 20°C	1/d
7	KHH20	KHH	2nd Order acid hydrolysis rate constant at 20°C	ℓ/mole-d
8	KHT	KHT	Temperature correction factor for hydrolysis	
9	XWSEG	WSEG	Number of water column segments	
10	HENRY	HNRY	Henry's Constant (set to zero to skip volatilization)	Unitless
11	MOLWT	MLWT	Molecular weight of toxicant	
12	KLT	KLT	Temperature correction factor for volatilization	

Required Constants (cont'd)

Constant	Fortran Variable Name	Suggested ANAME	Description	Units
13	ATMOS	ATMS	Concentration of chemical in the air immediately above the water	μg/ℓ
14	IFLOW	IFLW	Switch to indicate a flowing (0) or non-flowing (1) natural water system	
15	AIRTMP	ATMP	Air temperature	°C
16	A1	A1	Solids dependent partitioning exponent for solids type 1	
17	B1	B1	Solids dependent partitioning coefficient for for solids type 1	$1/\mathrm{mg}\cdot(\mathrm{mg}/\ell)^{A1}$
18	RHO1	RHO1	Density of solids type 1	gm/mℓ

IF ADDITIONAL SOLIDS TYPES ARE INCLUDED IN THE MODEL:

for each additional solids type add 3 parameters analogous to parameters 16, 17 and 18.

For example, if 2 solids types are considered (NOSYS=3) then constants 19 (A2), 20 (B2), and 21 (RHO2) must be included.

5.11 CARD GROUP I - MISCELLANEOUS TIME FUNCTIONS

The definition of miscellaneous piecewise linear time functions will vary depending upon the structure and the kinetics of the systems comprising each model. No time functions are currently considered and NFUNC should be set equal to zero. The user may wish to include time functions in a modified WASPB (e.g., temperature) and the input format is detailed below:

5.11.1 Number of Time Functions

5
NFUNC

FORMAT(I5)

NFUNC - number of time functions required for the model. If no time functions are to be inputted set NFUNC equal to zero and go to card group J.

5.11.2 Time Functions

The following package of cards is required for each time function. The first subpackage defines the function name and number of breaks in the time function. The second subpackage contains a detailed specification of the piecewise linear time function.

SubPackage I

4	10
ANAME(I)	NOBRK

FORMAT(A4,I6)

ANAME(I) - a one to four alpha-numeric character descriptive name for time function I.

NOBRK - number of breaks used to describe the time function I.

Sub-Package II

Each time series element consists of two parts; a function value and a time. The last card is a scale factor for the function value.

10	20	30	40	50	60	70	80
VALT(I)	T(I)	VALT(I+1)	T(I+1)	VALT(I+2)	T(I+2)	VALT(I+3)	T(I+3)

FORMAT(8F10.0)

VALT(I) - value of the function at time T(I).

T(I) - time in days; if the length of the simulation exceeds T(NOBRK), the time function will repeat itself, starting at T(1), i.e., the approximation is assumed to be periodic, with period equal to T(NOBRK). All time functions must have the same number of breaks and all break times must agree for all functions; i.e., T(1) must be the same for all functions, T(2) must be the same for all functions, etc.

2	15	35
OP	FACTOR	UNITS

FORMAT(A2,3X,F10.2,2A10)

OP - the operation (* / + - or **) of the scale factor.

FACTOR - the scaling value

UNITS - the units of time function after FACTOR has been applied.

5.12 CARD GROUP J - PHOTOLYSIS

1st order photolysis rate constants are computed for each water column segment in the model from the input indicated below: The calculation is adapted from Zepp and Cline (E,S & T, 11:359. 1977)

5.12.1. Execution switch

5
ISW
FORMAT(I5)

ISW = 0 - Photolysis is not considered and input is bypassed
1 - Photolysis included in model

5.12.2 Wavelengths for which data will be inputted

5
NOWAV
FORMAT(I5)

NOWAV = number of wavelengths considered.

Wavelengths are counted from a minimum wavelength of 297.5 nm in the following sequence:

297.5, 300, 302.5, 305, 307.5, 310, 312.5, 315, 317.5,
320, 323.1, 330., 340, 350, 360, 370, 380, 390, 400,
410, 420, 430, 440, 450, 460, 470, 480, 490, 500,
525, 550, 575, 600, 625, 650, 675, 700, 750, 800

NOWAV is thus controlled by the maximum wavelength at which the toxicant considered is photochemically active.

5.12.3 Toxicant Molar Absorptivity

```
          10         20
EPSILON(1)   EPSILON(2)    . . .       EPSILON(NOWAV)
FORMAT(8F10)
```

EPSILON(I) = molar absorptivity of the toxicant at wavelength number I ℓ/mole-cm

5.12.4 Toxicant quantum yield

```
        10
        QY
FORMAT(F10.)
```

QY = quantum yield of the toxicant

5.12.5 Location

```
        10        20        30
XLAT      XLONG     SEASON
FORMAT(3F10.)
```

XLAT = latitude of the natural water system being modeled (degrees)

XLONG = longitude of the natural water system being modeled (degrees)

SEASON = time of year:
1 - spring
2 - summer
3 - fall
4 - winter
5 - annual average

Note: if the system being modeled encompasses a wide range of latitude or longitude use average values in the model.

5.12.6 Water column light extinction

```
XKE(1)    XKE(2)     . . .     XKE(NOWAV)
```

XKE(I) = light extinction coefficient (1/meter) for wavelength number I

5.12.7 Effect of Cloud Cover

FCLOUD	BETA

FORMAT(2F10.)

FCLOUD = fraction of sky that is cloud covered
BETA = light reduction factor based on cloud type

Cloud type	BETA (avg. values)*
Cirrus	0.8 - 0.89
Cirrostratus	0.65 - 0.84
Altocumulus	0.45 - 0.52
Altostratus	0.41
Stratocumulus	0.31 - 0.35
Stratus	0.24 - 0.25
Fog	0.17 - 0.18

* Leighton, Photochemistry of Air Pollution, Academic Press, 1961.

5.13 CARD GROUP K - INITIAL CONDITIONS

5.13.1 Initial Conditions

5	15	20	30
ANAME(I)	C(ISYS,I)	ANAME(I+1)	C(ISYS,I+1)

35	45	50	60
ANAME(I+2)	C(ISYS,I+2)	ANAME(I+4)	C(ISYS,I+4)

FORMAT(4(A5,F10.0))

ANAME(I) - a one to five alpha-numeric character descriptive name the initial condition in segment I of system ISYS.

C(ISYS,I) initial condition in segment I of system ISYS in the appropriate units (normally mg/ℓ or ppm)

The user will be required to input initial conditions for each system even if the system is bypassed or if the initial conditions are zero. The initial conditions are read in one system at a time (from system 1 through system NOSYS), with concentrations being read from segment 1 through NOSEG within a segment package.

5.14 CARD GROUP L - STABILITY CRITERIA

10	20	30	....	80
CMAX(I)	CMAX(I+1)	CMAX(I+2)		CMAX(NOSYS)

FORMAT(8E10.0)

CMIN(I) - stability criteria for system I; i.e., the concentration (normal units mg/ℓ or ppm) above which program execution will be terminated because of probable numerical instability.

5.15 CARD GROUP M - PRINT CONTROL

5.15.1 Print Interval

10
P R N T

FORMAT(F10.0)

PRNT - print interval in days. (Set to zero for steady state option)

5.16 CARD GROUP N - INTEGRATION INFORMATION

5.16.1 Integration Interval, Total Time

10	20
DT	NTCHA

FORMAT(2F10.0)

For time variable option

DT - integration step size (normal units - days)

NTCHA - total time of time variable simulation

For steady state option

DT - set equal to 0.0

5.17 CARD GROUP O - DISPLAY PARAMETERS

All input is read NOSYS times, once for each system of the model. For each variable-segment combination chosen a time history of the segment will be displayed (dumped). For steady-state option no input is required; skip this card group.

5.17.1 Variable Names

8	16	80
ANAME(1)	ANAME(2)	ANAME(10)

FORMAT(10A8)

ANAME(K) = a one to eight alphanumeric character descriptive name for display variable K. The order of these names is determined via the appropriate disk file WRITE in the users kinetic subroutine 2.

5.17.2 Variable Number, Segment Numbers

3	6	9	27	31
VARNO	SEG(K)	SEG(K+1) ...	SEG(K+7)	ALLDMP

FORMAT(9I3,A4)

VARNO = the position of the desired variable, to be displayed, in the WRITE file statement in the kinetic subroutine (see previous note).

SEG(K) = segment number to be displayed (note: order of display unimportant, i.e., need not be sequential).

ALLDMP = flag set equal to ALL if all segments in the model are to be displayed.

A blank card terminates display for system, ISYS. Then, another Variable Name card, followed by Variable Number, Segment Number card(s) is read until system NOSYS has been read. NOTE: In the current version of the WASPB subroutine the variables written to output are:

VARNO	SYSTEM 1	SYSTEM 2
1	Total toxicant (μg/ℓ)	Solids concentration (mg/ℓ)
2	Dissolved toxicant (μg/ℓ)	
3	Particulate toxicant μg/g	

SECTION 6
EXAMPLE APPLICATIONS

6.1 KEPONE-JAMES RIVER, VA. (19)

The discharge of Kepone to the James River estuary from 1966 through 1975 resulted in widespread contamination of the estuarine system, extending the 120 kilometers from Hopewell, Virginia to the mouth of the James and into Chesapeake Bay. A model was developed to analyze the distribution of Kepone and project the time required to reduce concentrations to various levels. WASTOX was not available for use in the original work but was later applied to verify the original calculation.

To predict Kepone concentrations in the water column and sediment, the actual geomorphology, hydrology and tidal phenomena must be adequately reflected. To accomplish this, the water body must be divided into a sufficient number of segments so that each segment represents localized parameters of the system. In this way, variations of any parameter along the length of the river can be taken into account. Segment lengths must be short enough so that expected gradients in water and sediment concentrations can be accurately calculated.

With the above criteria in mind, the WASTOX version of the James River model was constructed of 74 completely mixed segments. The channel of the river consists of 56 segments and the four side bays and two tributaries of the river are represented by a total of 18 segments. Four layers of segments are used for the main channel, two in the water column and two in the sediment. In the more shallow side bays and tributaries, three vertical layers of segments are used, one for the water and two for the bed.

A schematic of an elevation view of the segments in the main channel is shown in the upper portion of Figure 3. Note that segments 1 through 28 define the two layers of the water column, segments 35 through 48 are in the first sediment layer and segments 55 through 68 constitute the second sediment layer.

The top sediment layer, subjected to horizontal movement by the lower water layer velocities, is referred to as the "moving sediment" layer or

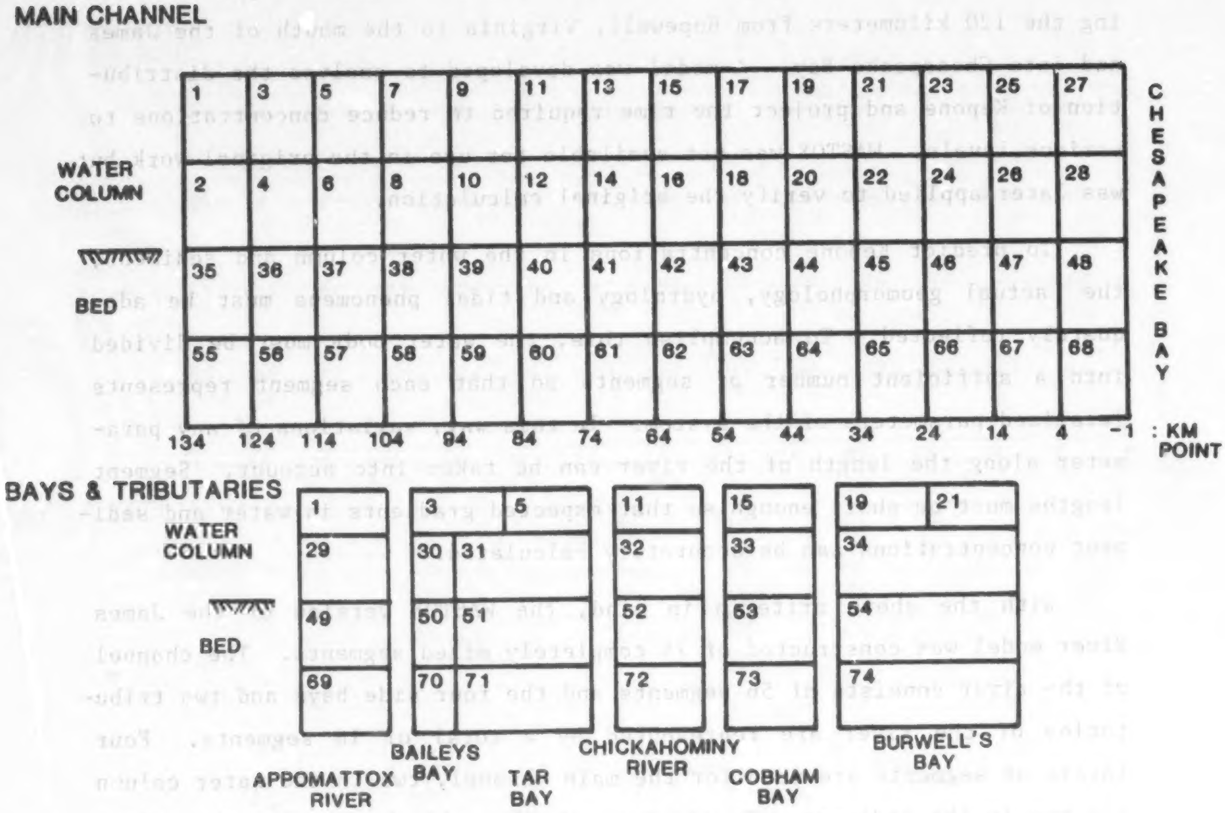

MAIN CHANNEL
WATER COLUMN
1 3 5 7 9 11 13 15 17 19 21 23 25 27
2 4 6 8 10 12 14 16 18 20 22 24 26 28
BED
35 36 37 38 39 40 41 42 43 44 45 46 47 48
55 56 57 58 59 60 61 62 63 64 65 66 67 68
CHESAPEAKE BAY
134 124 114 104 94 84 74 64 54 44 34 24 14 4 −1 : KM POINT
BAYS & TRIBUTARIES
WATER COLUMN
BED
1 29 49 69
3 5 30 31 50 51 70 71
11 32 52 72
15 33 53 73
19 21 34 54 74
APPOMATTOX RIVER
BAILEYS BAY
TAR BAY
CHICKAHOMINY RIVER
COBHAM BAY
BURWELL'S BAY

FIGURE 3. SEGMENTATION OF THE JAMES RIVER USED IN THE KEPONE ANALYSIS

the "moving bed" and the second sediment layer is the "stationary bed". As shown in the lower portion of the figure, segments 29 through 34 are the water segments, sequentially numbered, in the Appomattox River, Baileys Bay, Tar Bay, Chickahominy River, Cobham Bay and Burwell Bay. For the same locations, segments 49 through 54 and 69 through 74 represent the moving and stationary bed segments, respectively.

In the main channel, segment lengths are all approximately 10 kilometers long. With 14 segments end-to-end, the model represents 135 kilometers of river from its mouth to above Hopewell.

The water column was divided into two layers to account for the net tidal flow profile in the estuary in which high salinity water moves upstream in the lower layer and less dense low salinity water moves downstream in the upper layers. The depths of the two layers were defined by the plane of no net motion, i.e., the location of zero velocity where the flow direction changes. Based on available sediment data, depths of 10 and 30 centimeters were selected for the moving and stationary beds, respectively.

The analysis procedure, which is appropriate for those cases in which the system has been previously subjected to an input of a toxic substance, essentially consisted of four steps, shown diagrammatically in Figure 4. First, equations of continuity, momentum and state were employed in a steady-state tidally averaged mode to generate the horizontal and vertical velocities of the estuarine circulation. A steady state model of the water column was then used to determine the vertical dispersion coefficient between the two water layers using ocean salt as a tracer. Secondly, settling velocities of solids to the bed and resuspension of solids from the bed were estimated to match observed solids concentration in the water column. A settling velocity was assigned and assuming a surface bed solids concentration of 50,000 mg/ℓ the resuspension velocities needed to match suspended solids concentrations were determined. These velocities were checked by calculating the dissolved and particulate organic Kepone concentrations in the water column using the observed Kepone concentrations in the surficial sediments as a boundary condition. From this procedure a settling velocity of 4 ft/d (1.2 m/d) was assigned as characteristic of the James River solids.

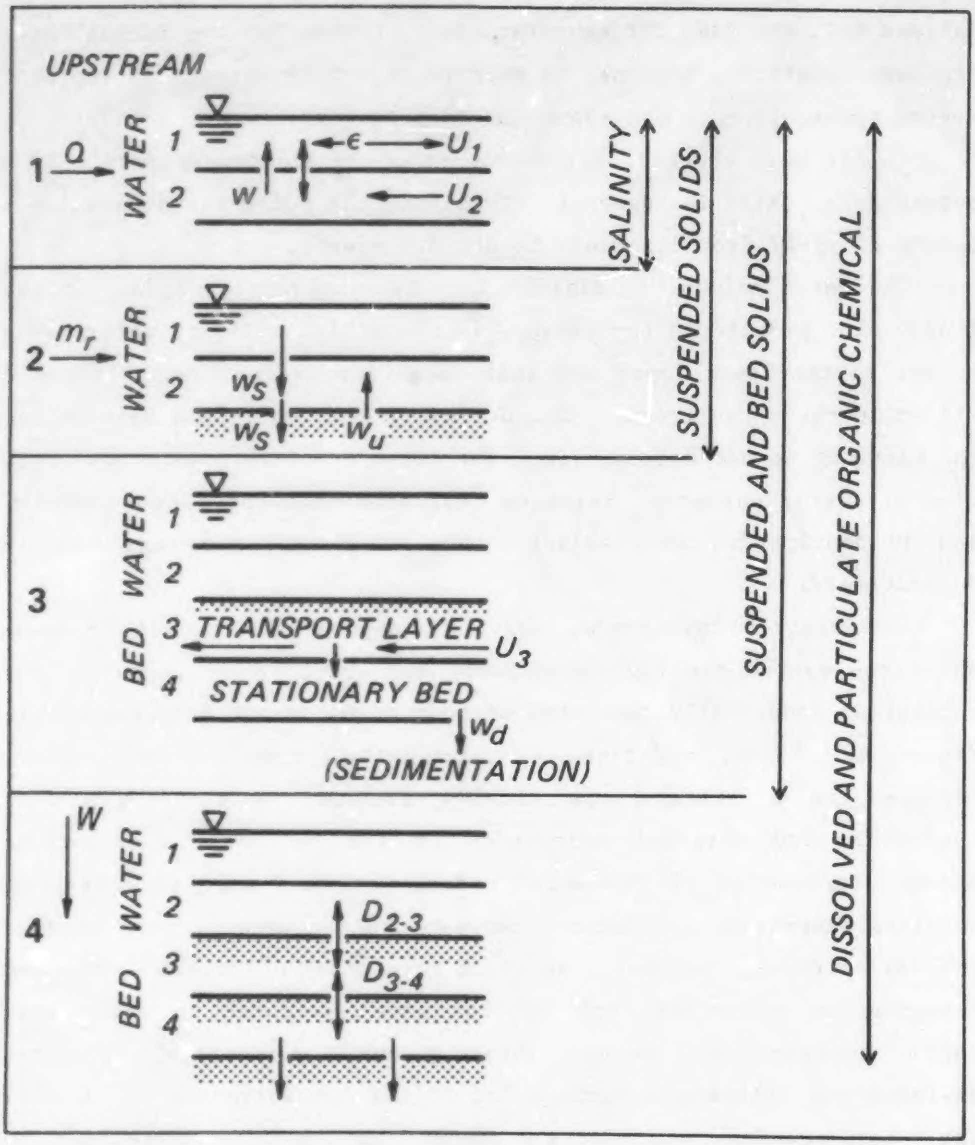

UPSTREAM
1
Q
WATER
1
2
w
ϵ
U_1
U_2
SALINITY
2
m_r
WATER
1
2
w_s
w_s
w_u
SUSPENDED SOLIDS
3
WATER
BED
1
2
3
4
TRANSPORT LAYER
U_3
STATIONARY BED
w_d
(SEDIMENTATION)
SUSPENDED AND BED SOLIDS
4
W
WATER
BED
1
2
3
4
D_{2-3}
D_{3-4}
DISSOLVED AND PARTICULATE ORGANIC CHEMICAL

FIGURE 4. SEQUENCE OF STEPS IN JAMES RIVER USED IN THE KEPONE ANALYSIS(23)

In the third step, the solids transport in the bed was addressed. Net horizontal velocities of the transport layer were assigned and the flux of sediment between the two sediment layers was determined by mass balance. With selected values of solids concentrations for both the transport and stationary beds of 50,000 and 500,000 mg/ℓ respectively and the settling and resuspension rates from step two, the net sedimentation rate of the bed was calculated and compared to observed rates in the estuary.

The last step consisted of calculating the dissolved and particulate concentrations of Kepone in the water and bed. The diffusivity of the dissolved component in the interstitial water was assigned as 5×10^{-6} cm^2/s. A solids dependent sorption partition coefficient was used.

The Kepone distribution in the water and the bed were first calculated for various freshwater flows held constant over the period of analysis. The actual hydrograph for the time period beginning in 1965 was then approximated by six constant flow conditions and the Kepone distribution calculated. WASTOX has been applied only to the constant flow condition although it could also be used for the variable flow simulation.

The results of the model for a freshwater flow of 1000 cfs are shown in Figure 5.

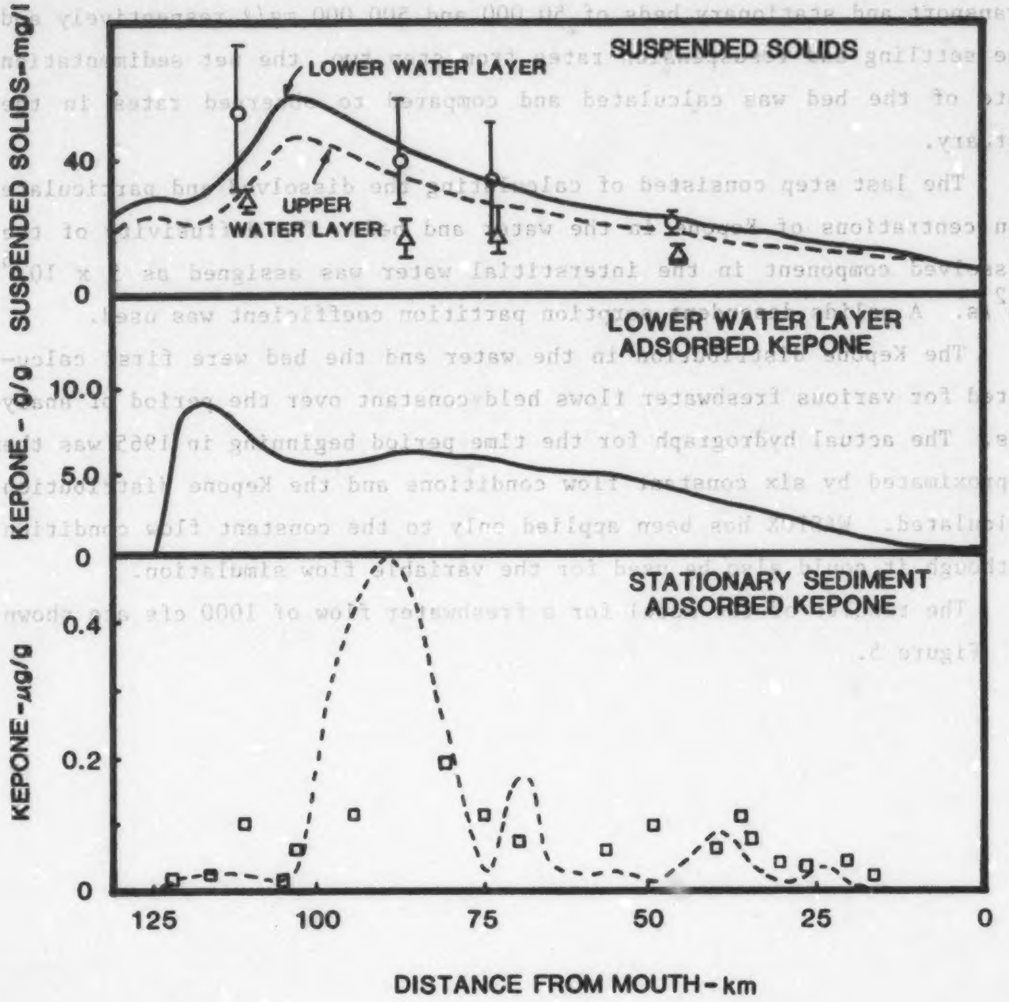


FIGURE 5. COMPARISON OF OBSERVED AND COMPUTED SUSPENDED SOLIDS AND KEPONE FOR THE 1000 CFS FRESHWATER FLOW

6.2 PLUTONIUM-239, PCB - GREAT LAKES (21)

The Great Lakes represent the major fresh water resource of the United States as well as one of the major resources for Canada. Because of the significance of these bodies of water, there is a unique and long term concern over the fate of chemicals that may be potentially toxic to the aquatic ecosystem as well as to the general public health. The discharge of chemicals such as the heavy metals including mercury, and organic chemicals such as polychlorinated biphenyls (PCB) and mirex have resulted in the closing of commercial and sports fishing opportunities. As a result of these concerns, a need exists to develop a framework for the Great Lakes that would permit estimates to be made of the fate of chemicals discharged to the Lakes.

WASTOX was used for the calculations associated with a physico-chemical model of the Great Lakes system. Full details of the model, calibration and application to chemical fate in the Great Lakes is given in Thomann and Di Toro (21).

The time scale of the model is considered to be long term, i.e. year to year. The physical segmentation of the model considers the Lakes to be completely mixed with the exception of Lake Erie (Figure 6). This Lake is divided into three basins; west, central, and east to reflect varying regions of solids deposition and water column solids concentrations. In addition, Saginaw Bay is included as a separate embayment from Lake Huron to represent a more local region interacting with a large lake. Three sediment segments of 2 cm each in depth are included under each of the lakes or region of lake. This results in a model with eight water column segments and twenty-four sediment segments for a total of thirty-two segments.

The calibration procedure was as follows: (a) From a review of data on fine grain solids loading to the Lakes, net depositional flux of solids, and water column suspended solids concentrations, the net loss rate of solids from the water column was estimated. From assigned porosity in the surface sediment layer, particle density and net flux of solids to the sediment, the net sedimentation rate is computed. (b) With the estimate of the net loss of solids, w_n, a range of particle settling velo-

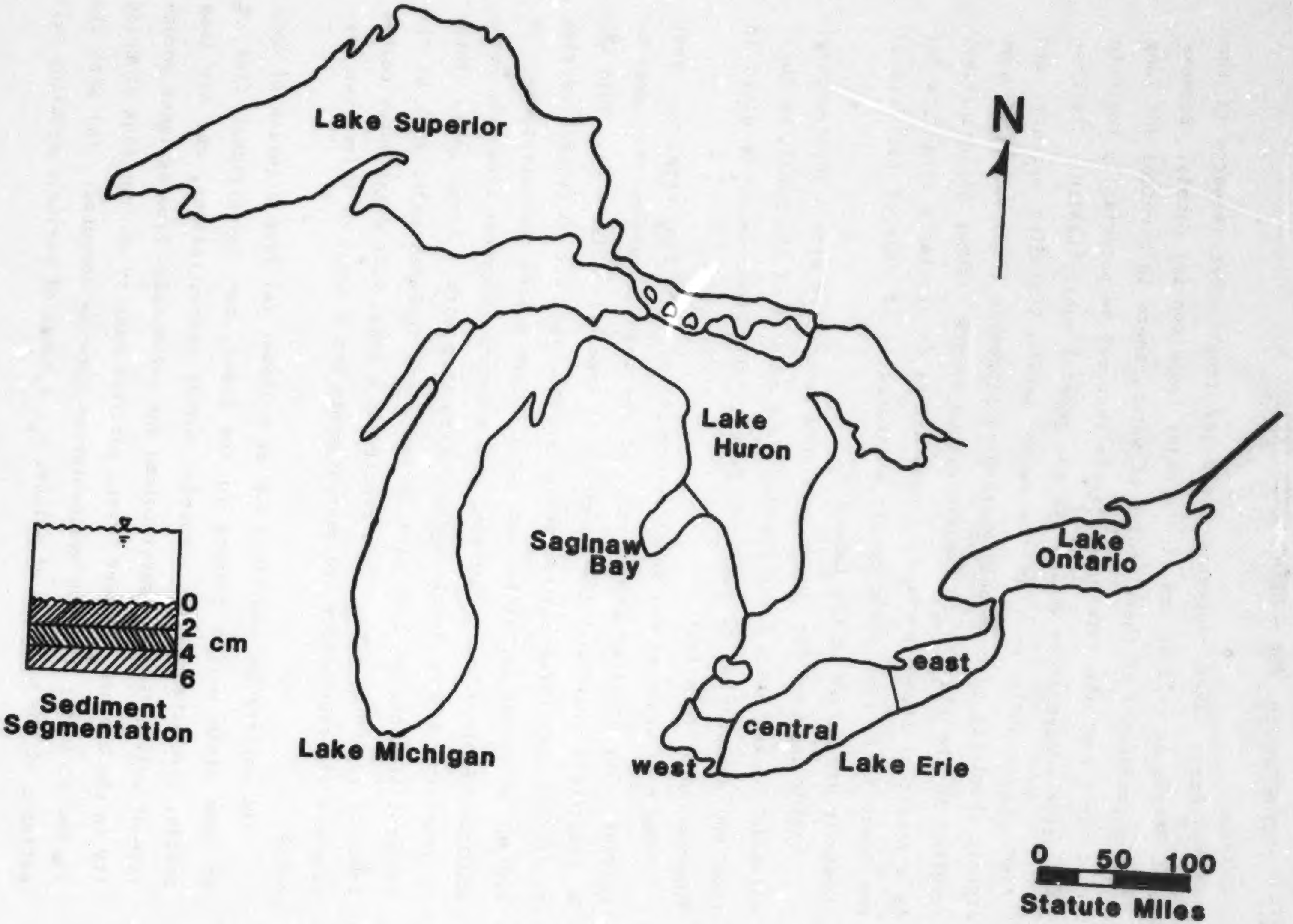

Lake Superior
N
Lake Huron
Saginaw Bay
Lake Ontario
Lake Michigan
east
central
west
Lake Erie
0
2
4
6
cm
Sediment Segmentation
0 50 100
Statute Miles

FIGURE 6. SEGMENTATION OF THE GREAT LAKES AND SAGINAW BAY

cities were assigned and the resuspension velocity necessary to maintain the solids balance was computed. (c) Since there is an infinite number of combinations of settling and resuspension velocities that will result in the same solids balance, a time variable plutonium-239 model was used to provide the tracer calibration. All decay mechanisms and sediment diffusion were assumed to be zero and a sensitivity analysis using three values of plutonium solids partitioning was conducted.

Following calibration of the model using plutonium-239 as a tracer, the model was applied to PCB, benzo(a) pyrene and cadmium.

The comparisons of observed plutonium-239 data in the 1970's to model calculations are shown in Figure 7 (w_a = particle settling velocity, w_{net} = net loss of solids, $w_a = w_{net}$ indicates zero resuspension). The calibration indicated that in general the sediments are interactive with the water column in the Great Lakes through resuspension and/or horizontal transport.

The results of the application of the model to PCB using a 20 year calculation indicate that a load level ranging from 640 to 1390 kg/yr with volatilization (at an exchange rate of 0.1 m/d) appears to be representative of observed surface sediment data for the open lake waters (Figure 8). Fifty percent response times for PCB following cessation of load and including volatilization varied from less than 5 years to 10-20 years for the other lakes without volatilization. Comparison of these response times to decline of concentrations of PCB in Lake Michigan indicates that at least for that lake volatilization is occurring at an exchange rate of about 0.1 m/d.

6.3 PENTACHLOROPHENOL - EPA MERS CHANNELS (22)

Pentachlorophenol (PCP) and its salts have historically been used for the preservation and treatment of wood. However, their antimicrobial, antifungal, herbicidal and insecticidal properties have led to widespread application of PCP. Increased knowledge of the behavior and fate of PCB in the aqueous environment will enable its impact to be effectively managed. During 1982 EPA executed a PCP fate and effects study utilizing the semi-natural stream channels at the Monticello Environmental Research Laboratory. The 1400 ft. channels consist of alternative pool and riffle

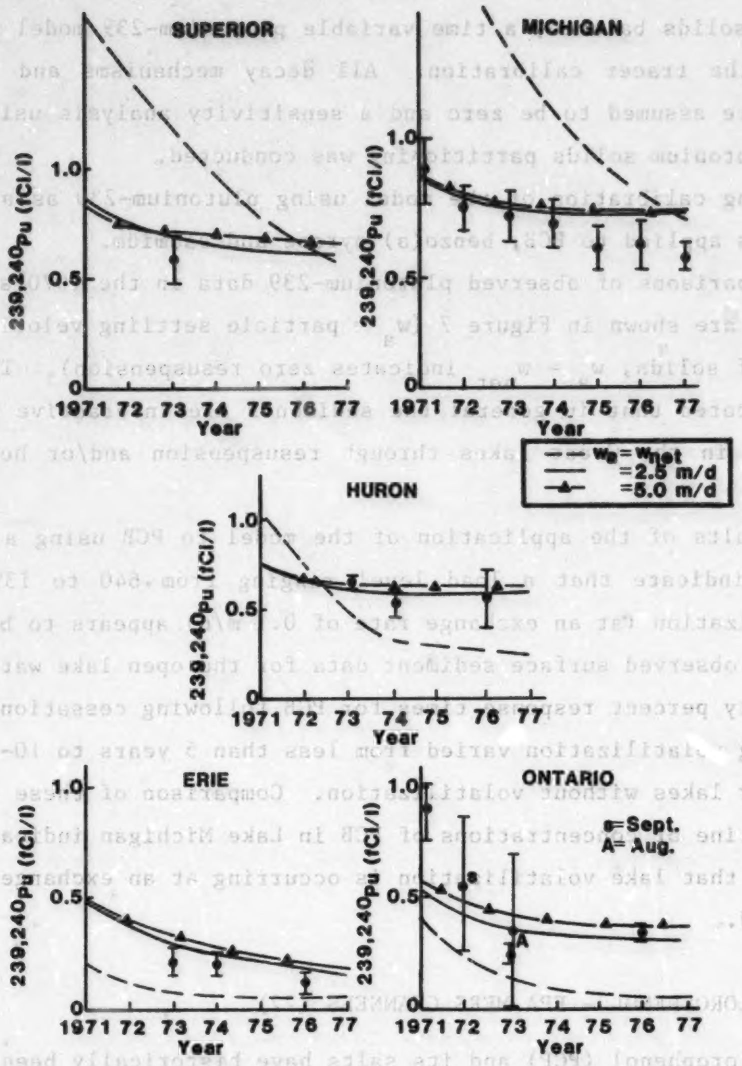


FIGURE 7. COMPARISON OF 1971-1977 OBSERVED AND CALCULATED WATER COLUMN ^{239,240}Pu CONCENTRATION FOR THREE CONDITIONS OF THE PARTICULATE SETTLING VELOCITY.

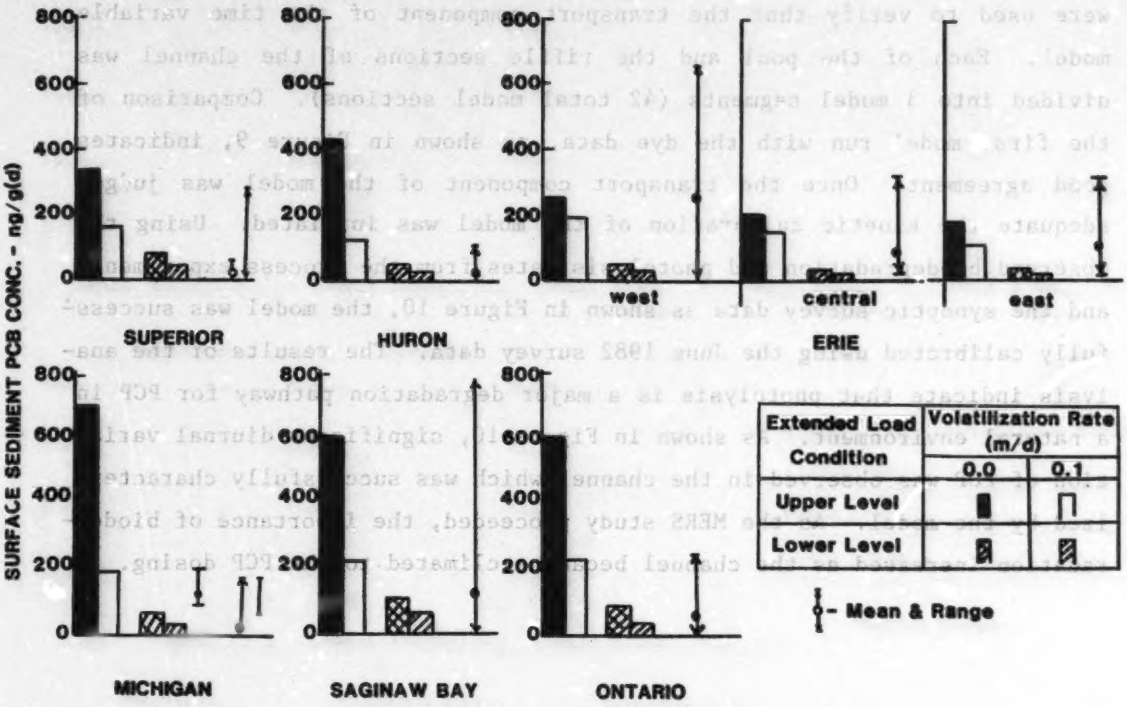


FIGURE 8. CALCULATED SUERFACE SEDIMENT PCB CONCENTRATION (ng/g) FOR CONDITIONS ON EXTERNAL BED AND VOLATILIZATION RATE AND COMPARISON TO OBSERVED DATA

sections and during the study a constant 0.45 cfs (0.013 m^3/s) flow was maintained. Process experiments to quantify photolysis and biodegradation decay rates, two comprehensive survey data sets and the results of a dye study were utilized to construct and calibrate a mathematical model of the transport and fate of PCP in the channels. Manhattan College's toxic substance computer program (WASTOX) was used as the modeling framework.

Since photolysis was a major degradation mechanism for PCP, a time variable model was constructed which utilized observed hourly solar radiation measurements. The results of a detailed travel time/dispersion study were used to verify that the transport component of the time variable model. Each of the pool and the riffle sections of the channel was divided into 3 model segments (42 total model sections). Comparison of the first model run with the dye data, as shown in Figure 9, indicates good agreement. Once the transport component of the model was judged adequate the kinetic calibration of the model was initiated. Using the observed biodegradation and photolysis rates from the process experiments and the synoptic survey data as shown in Figure 10, the model was successfully calibrated using the June 1982 survey data. The results of the analysis indicate that photolysis is a major degradation pathway for PCP in a natural environment. As shown in Figure 10, significant diurnal variation of PCP was observed in the channel which was successfully characterized by the model. As the MERS study proceeded, the importance of biodegradation increased as the channel became acclimated to the PCP dosing.

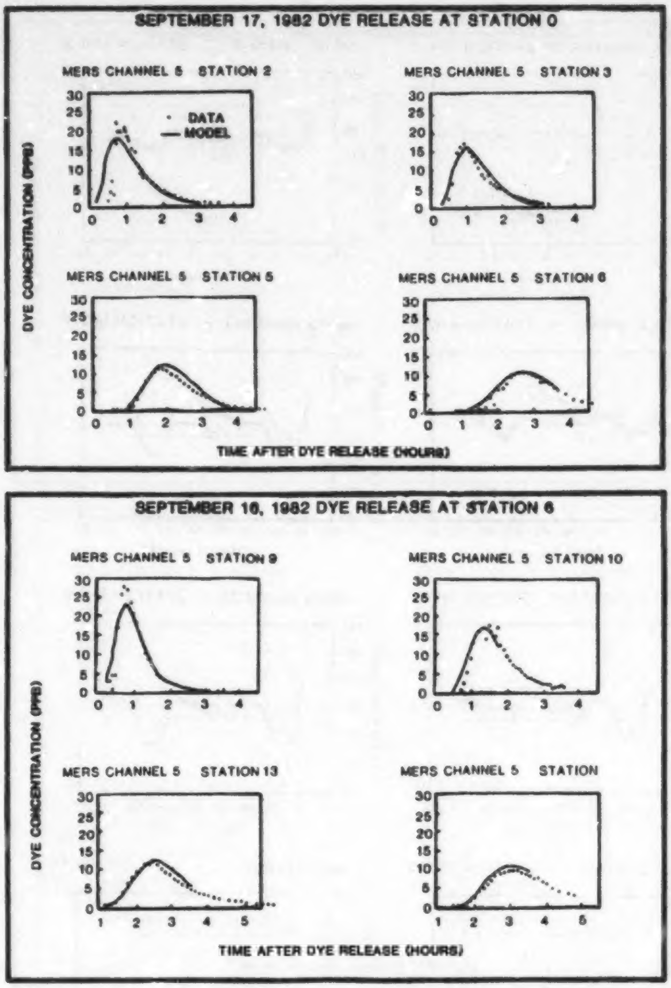


FIGURE 9: Model Comparison with September 16 and 17 Rhodamine WT Dye Data.

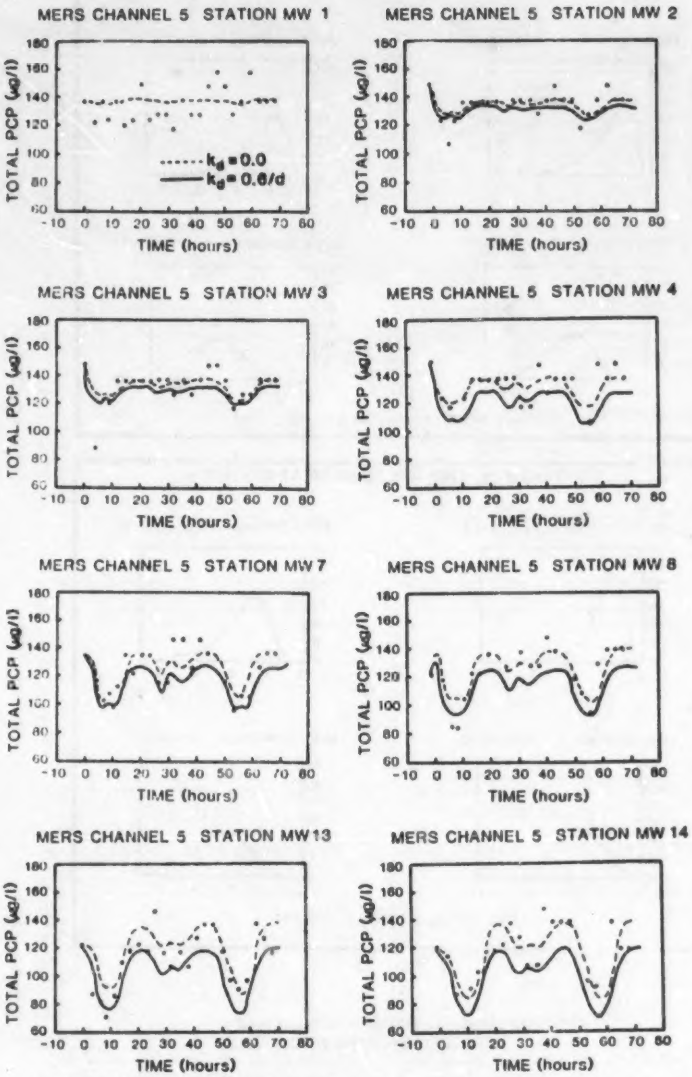


FIGURE 10: Time Variable Model Comparison with MERS Channel J
Total PCP data - Stations 1, 2, 3, 4, 5, 6, 7, 8, 13, 14
June 8 to 10, 1982

SECTION 7
OPERATIONAL CONSIDERATIONS

This chapter describes how to obtain the computer program WASTOX, how to install it on a DEC PDP mini computer, how to test the program with a sample dataset, and what machine limitations limit the program.

7.1 AQUISITION PROCEDURES

To obtain the program WASTOX along with a sample dataset and support software, write to:

Center for Water Quality Modeling
Environmental Research Laboratory
U.S. Environmental Protection Agency
College Station Road
Athens, GA 30613

A nine-track magnetic tape will be mailed to you. Please copy the contents and return the tape.

7.2 INSTALLATION PROCEDURES

The subroutines that comprise WASTOX must be compiled and linked into a task image. This is accomplished on the PDP IAS operating system by running the command file "WXTCMP.CTL." If the compilation succeeds, then linkage is automatically attempted with the command file "WXTLNK.CTL."

7.3 TESTING PROCEDURES

Once WASTOX is installed, the sample input dataset should be run and compared with the sample output dataset to verify that the program is calculating correctly. To perform a simulation on the PDP, submit the batch input sequence "WXTRUN.CTL."

7.4 MACHINE LIMITATIONS

Currently, TOXIWASP is set up for the following configuration:

PDP 11/70 Hardware
RSTS/E operating system
FORTRAN IV

60 segments - steady-state

75 segments - time-variable
4 systems

The PDP 11/70 computer utilizing RSTS/E operating system allocates a 32k word (64k byte) user area for execution of programs. WASTOX occupies at least 31k words of memory. Any enlargement of this program may result in an overflow of the user area.

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APPENDIX 1

GLOSSARY OF VARIABLES

I. Variables in Common Block MAIN

BBC - Matrix of order (NOSYS, Max. No. of boundaries per system)
Contains the boundary concentrations in mg/ℓ.

BQ - Vector of length (Max. No. of Flows)
Contains flows in 10^6 ft^3/d.

BR - Vector of length (Max. No. of exchanges)
Contains the exchanges in 10^6 ft^3/d.

BVOL - Vector of length (NOSEG)
Contains the segment volumes in 10^6 ft^3

BWK - Matrix of order (NOSYS, Max. No. of loads per system)
Contains the loadings or discharge rates in lb/d.

C - Matrix of order (NOSYS, NOSEG)
Contains the current concentrations for each system and segment in mg/ℓ-d.

CD - Matrix of order (NOSYS, NOSEG)
Contains the current time derivative for each system and segment in mg/ℓ-d.

CMAX - Vector of length (NOSYS)
Contains the maximum allowable concentration for each system in mg/ℓ.

CONST - Vector of length (Max. No. of Constants)
Contains the kinetic coefficients used in WASPB

DT - Integration interval in days.

IBC - Matrix of order (NOSYS, Max. No. of boundaries per system)
Contains the segment numbers for the corresponding boundary concentrations in BBC.

IBCOP - Vector of length (NOSYS)
Contains the option numbers for inputting boundary concentrations.

IQ - Vector of length (Max. No. of Flows)
Contains the numbers of the segments to which flow is directed for the corresponding flows in BQ.

IQOPT - Option number for inputting flows.

IR - Vector of length (Max. No. of Exchanges)
Contains the segment numbers for the first segment corresponding to the exchanges in BR

IROPT - Option number for inputting exchanges.

ITIMB - Vector of length (NOSYS)
Counter for time variable boundary conditions.

ITIMD - Counter for time variable dispersions.

ITIMF - Counter for time variable straight line functions.

ITIMQ - Counter for time variable flows.

ITIMR - Counter for time variable exchanges.

ITIMV - Counter for time variable volumes.

ITIMW - Vector of length (NOSYS)
Counter for time variable forcing functions.

IVOPT - Option number for inputting volumes.

IWK - Matrix of order (NOSYS, Max. No. of loads per system)
Contains the numbers of the segments in which the corresponding discharges in BWK are occurring.

IWKOP - Vector of length (NOSYS)
Contains the option number for inputting discharges or (forcing functions).

JQ - Vector of length (Max. No. of Flows)
Contains the numbers of the segments from which flow is leaving for the corresponding flows in BQ.

JR - Vector of length (Max. No. of Exchanges)
Contains the segment numbers for the second segment corresponding to the exchanges in BR.

MBC - Matrix of order (NOSYS, Max. No. of boundaries per system)
For a time-varying boundary concentration MBC contains the current slope of the broken line approximation. For a time-varying option BBC contains the intercept of the current line segment of the broken line approximation.

MQ - Vector of length (Max. No. of flows)
Slope for time-varying flows analogous to MBC.

MR - Vector of length (Max. No. of Exchanges)
Slope for time-varying exchanges analogous to MBC.

MVOL - Vector of length (NOSEG)
Slope for time-varying segment volumes analogous to MBC.

MWK - Matrix of order (NOSYS, Max. No. of Loads per system)
Slope for time-varying loads or (forcing functions) analogous to MBC.

NFUNC - No. of user defined broken line functions.

NFUNT - Time of next break in user defined broken line functions in days.

NOBC - Vector of length (NOSYS)
Contains the number of boundary conditions for each system.

NOQ - Contains the number of flows for a particular flow field.

NOR - Contains the number of exchanges for a particular exchange field.

NOWK - Vector of length (NOSYS)
Contains the number of loads (forcing functions) for each system.

NQT - Time of next break in flow broken-line function in days.

NRT - Time of next break in exchange broken-line function in days.

NTCHA - Total time of run in days.

NVOLT - Time of next break in segment volume broken-line function in days.

NWKT - Vector of length (NOSYS)
Contains the time of the next break in the forcing function broken-line function for each system in days.

PARAM - Matrix of order (NOSEG, Max. No. of parameters per segment)
Contains the values for each segment of the parameters used in WASPB.

PRNT - Print interval in days.

TIME - Current time in days.

II. Variables in Common Block SYSTRN

FIELDQ - Vector of length (Max. No. of flow fields)
Contains the number of flows read in for the current and all prior flow fields.

FIELDR - Vector of length (Max. No. of exchange fields)
Contains the number of exchanges read in for the current and all prior exchange fields.

FPART - Matrix of order (NOSYS, NOSEG)
Contains the fraction of total chemical in each segment that is dissolved or adsorbed to the solids of each system.

SCALEQ - Matrix of order (NOSYS, Max. No. of flow fields)
Contains the scale factors by which the flows in each flow field are multiplied for each system.

SCALER - Matrix of order (NOSYS, Max. No. of exchange fields)
Contains the scale factors by which the exchanges in each flow field are multiplied for each system.

III. Variables in Common Block MAINA

IN - Unit number designation for input.

IREC - Counter for number of times results are written to disk.

IRECL - Vector of length (NOSYS)
Contains the record number of the first record of the results on disk for a specific time.

ISYS - Current system being processed.

NOSEG - Number of segments in the model.

OUT - Unit number designation for output.

SYSEXC - Vector of length (NOSYS)
Contains the system bypass option for each system.

IV. Variables in Common Block PHOTO

DAYK - Vector of length (NOSEG)
Contains the photolysis rate constants for each segment.

V. Variables in Common Block COMP

BFUNC - Vector of length (Max. no. of user defined broken-line functions)

IEV - Switch to indicate to WASP8 which input broken-line function is being evaluated.

ITIME - Counter for user defined broken-line functions.

MFUNC - Vector of length (Max. no. of user defined broken-line functions)
Contains the current slope of each broken-line function.

NBCT - Vector of length (Max. no. of boundary conditions)
Time of next break in each boundary condition broken-line function.

NDEVL - Switch to indicate time for writing results on disk.

VI. Variables in Common Block DUMP

MXDMP - Number of variables written to disk for each system each time results are dumped.

MXSEG - Maximum number of segments allowed in the model.

VII. Local variables in the kinetic subroutine WASPB

A1,A2,A3 - Solids dependent adsorption experiment for solids type 1,2, or 3.

ATMOS - Concentration of chemical in the air above the water body in ____.

AREA - Vector of length (NOSEG)
Area of each segment at its downstream face in ft^2.

B1,B2,B3 - Solids dependent adsorption coefficient for solids type 1,2, or 3.

BACS1 - Vectors of length (NOSEG)

BACS2 - Concentration of compound degrading bacteria on solids type.

BACS3 - 1,2, or 3 in num/mg.

BACW - Vector of length (NOSEG)
Concentration of compound degrading bacteria in water in num/ℓ.

BIOS - Vector of length (NOSYS-1)
Computed rate of biodegradation on each solids type in µg/ℓ-d.

BIOW - Computed rate of biodegradation in water in µg/ℓ-d.

DEPTH - Vector of length (NOSEG)
Depth of each segment in meters

DIFF - Molecular diffusivity of chemical in m^2/s

DISTOX - Concentration of dissolved chemical in µg/ℓ

DTIME - Time between current time and next break in user defined broken-line approximation.

DVMMY - Extra variable used when results are written to disk to keep the number of variables written for each system equal to MXDMP when less than MXDMP variables are needed for a system.

DWNSEG - Vector of length (NOSEG)
Number of segment downstream of each segment.

H - Hydrogen ion concentration in moles/ℓ.

HENRY - Henry's Constant - unitless.

HYDROL - Computed hydrolysis rate in μg/ℓ for dissolved chemical

IFLOW - Switch to indicate a flowing(0) or non-flowing(1) water body.

KD - Biodegradation second order rate constant for dissolved chemical in ℓ/d-num.

KDI - Temperature correction factor for biodegradation of dissolved chemical.

KD20 - Biodegradation second order rate constant for dissolved chemical at 20°C in ℓ/d-num.

KH - Total hydrolysis rate constant in 1/d.

KHH - Acid hydrolysis second order rate constant in ℓ/d-mole.

KHH20 - Acid hydrolysis second order rate constant at 20°C in ℓ/d-mole.

KHN - Neutral hydrolysis first order rate constant in 1/d.

KHN20 - Acid hydrolysis second order rate constant at 20°C in ℓ/d-mole.

KHOH - Alkaline hydrolysis second order rate constant in ℓ/d-mole.

KHT - Temperature correction factor for hydrolysis.

KL - Volatilization rate constant in m/d.

KLA - Volatilization rate constant in 1/d.

KLT - Temperature correction factor for volatilization.

KP - Biodegration second order rate constant for adsorbed chemical in ℓ/d-num.

KPT - Temperature correction factor for biodegradation of adsorbed chemical.

KP20 - Biodegradation second order rate constant for adsorbed chemical at 20°C in ℓ/d-num.

MOUNT - Molecular weight of chemical

OH - Hydroxide ion concentration in moles/ℓ

PART - Vector of length (NOSYS)
Partition coefficient for each system in ℓ/mg

PARTOX - Vector of length (NOSYS-1)
Concentration of adsorbed chemical for each solids type in μg/ℓ

PH - Vector of length (NOSEG)
pH of each segment

PHOTOL - Photolysis rate in μg/ℓ-d

PORE - Porosity of a segment

RHO - Vector of length (NOSYS-1)
density of each solids type in g/mℓ

TDEPTH - Vector of length (NOSEG)
Depth from the water surface of the top of the segment in meters

TEMP - Vector of length (NOSEG)
Temperature of each segment in °C

VEL - Flow velocity in m/s

VOLAT - Volatilization rate in μg/ℓ-d
XKGH - Gas film transfer coefficient
XKL - Liquid film transfer coefficient

APPENDIX 2

Listing of Kinetic Subroutine WASPB

```
0001        SUBROUTINE WASPB
      C
      C      THIS MODEL IS SET UP TO COMPUTE THE SPATIAL AND TEMPORAL
      C      DISTRIBUTION OF TOXIC CHEMICALS IN ESTUARIES.  IT MODELS
      C      TOTAL TOXICANT AND UP TO 3 CLASSES OF SOLIDS.  THE DISTRIBUTION
      C      OF TOXICANT BETWEEN THE DISSOLVED AND VARIOUS PARTICULATE
      C      PHASES IS COMPUTED FROM THE TOTAL TOXICANT ASSUMING
      C      INSTANTANEOUS EQUILIBRIUM LINEAR PARTITIONING.
      C
      C
      C      SYSTEM 1 IS TOTAL TOXICANT
      C      SYSTEMS 2 THROUGH N ARE SOLIDS
      C
      C
      C
      C
      C    ********************************************************************
      C    *                                                                  *
      C    *                 < < < < < C O M M O N > > > > >                  *
      C    *                                                                  *
      C    *                                                                  *
      C    *                                                                  *
      C    *                                                                  *
      C    *     THIS MODEL IS DIMENSIONED FOR THE FOLLOWING:                 *
      C    *                                                                  *
      C    *         4  SYSTEMS                                               *
      C    *        75  SEGMENTS                                              *
      C    *       100  EXCHANGES                                             *
      C    *       200  FLOWS                                                 *
      C    *        50  BOUNDARIES                                            *
      C    *        17  FORCING FUNCTIONS                                     *
      C    *        11  SYSTEM PARAMETERS                                     *
      C    *        30  CONSTANTS                                             *
      C    *         4  STRAIGHT LINE FUNCS                                   *
      C    *         9  FLOW FIELDS                                           *
      C    *         9  EXCHANGE FIELDS                                       *
      C    *                                                                  *
      C    *                                                                  *
      C    *                                                                  *
      C    *                                                                  *
0002        COMMON /MAIN/                                                     *
           *   BBC( 4,50), BQ(200),    BR(100),    BVOL( 75),  BWK( 4, 17),   *
           *   C( 4, 75),  CD( 4, 75), CMAX( 4),   CMIN( 4),   CONST(30),     *
           *   DT,         IBC( 4,50), IBCOP( 4),              IQ(200),       *
           *   IQOPT,      IR(100),    IROPT,      ITIMB( 4),  ITIMD,         *
           *   ITIMF,      ITIMQ,      ITIMR,      ITIMV,      ITIMW( 4),     *
           *   IVOPT,      IWK( 4, 17), IWKOP( 4),  JQ(200),    JR(100),      *
           *   MBC( 4,50), MQ(200),    MR(100),    MVOL( 75),  MWK( 4, 17),   *
           *   NFUNC,      NFUNT,      NOBC( 4),   NOQ,        NOR,           *
           *   NOWK( 4),   NQT,        NRT,        NTCHA,      NVOLT,         *
           *   NWKT( 4),   PARAM( 75,11),PRNT,                                *
           *   TIME                                                           *
      C    *                                                                  *
0003        REAL                                                              *
```

```
           *   MBC,        MQ,         MR,         MVOL,       MWK,            *
           *   NFUNT,      NQT,        NRT,        NTCHA,      NVOLT,          *
           *   NWKT                                                            *
      C    *                                                                   *
      C    *                                                                   *
0004        COMMON /MAINA/                                                     *
           *   IN,         IREC,       IRECL( 4),              ISYS,           *
           *   NOSEG,      NOSYS,      OUT,                  SYSEXC( 4)    *
      C    *                                                                   *
0005        INTEGER                                                            *
           *   OUT,                    SYSEXC                                  *
      C    *                                                                   *
      C    *                                                                   *
0006        COMMON /COMP/                                                      *
           *   BFUNC(  4), IEV,        ITIME,      MFUNC(  4), NBCT( 4),       *
           *   NDEVL                                                           *
      C    *                                                                   *
0007        REAL                                                               *
           *   MFUNC,      NBCT,       NDEVL                                   *
      C    *                                                                   *
      C    *                                                                   *
0008        COMMON /SYSTRN/                                                    *
           *   SCALEQ(  4, 9),SCALER(  4, 9),FIELDQ,FIELDR                     *
           *   ,FPART( 4, 75)                                                  *
      C    *                                                                   *
0009        INTEGER                                                            *
           *   FIELDQ( 9),FIELDR( 9)                                           *
      C    *                                                                   *
      C    *                                                                   *
      C    *                                                                   *
      C    *********************************************************************
      C
0010        COMMON /DUMP/ MXDMP, MXSEG
      C
      C*************************************************************************
      C
      C          DESCRIPTION OF PARAMETERS AND CONSTANTS
      C
      C*************************************************************************
      C
      C  PARAM NAME          DESCRIPTION                             UNITS
      C
      C   DEPTH       DEPTH OF THE SEGMENT                          METERS
      C   TDEPTH      DEPTH FROM THE WATER SURFACE OF THE
      C               TOP OF THE SEGMENT                            METERS
      C   DWNSEG      SEGMENT DOWNSTREAM OF THE CURRENT SEGMENT
      C   AREA        AREA BETWEEN THE CURRENT SEGMENT AND THE
      C               DOWNSTREAM SEGMENT                             FT**2
      C   PH          PH OF THE SEGMENT
      C   TEMP        TEMPERATURE OF THE SEGMENT                  CENTIGRADE
      C   WVEL        WIND VELOCITY ABOVE THE SEGMENT                  M/S
      C   BACW        CONCENTRATION OF BACTERIA IN THE WATER        NUM/L
      C   BACSI       CONCENTRATION OF BACTERIA ON SOLIDS
      C                TYPE I                                      NUM/MG
      C
      C
      C  CONST NAME          DESCRIPTION                              UNITS
      C
      C     KD20      2ND ORDER BIODEGRADATION RATE CONSTANT
      C               FOR DISSOLVED TOXICANT AT 20 DEGREES C          L/D-NUM
      C     KDT       TEMP. CORRECTION FACTOR FOR BIODEGRA-
      C               DATION OF DISSOLVED TOXICANT
      C     KP20      2ND ORDER BIODEGRADATION RATE CONSTANT
      C               FOR SORBED TOXICANT                             L/D-NUM
      C     KPT       TEMP. CORRECTION FACTOR FOR BIODEGRA-
      C               DATION OF SORBED TOXICANT
      C     KHOH20    2ND ORDER ALKALINE HYDROLYSIS RATE
      C               CONSTANT AT 20 DEGREES C                       L/MOLE-D
      C     KHN20     1ST ORDER NEUTRAL HYDROLYSIS RATE
      C               CONSTANT AT 20 DEGREES C                        1/DAY
      C     KHH20     2ND ORDER ACID HYDROLYSIS RATE CONSTANT
      C               AT 20 DEGREES C                                L/MOLE-D
      C     KHT       TEMP. CORRECTION FACTOR FOR HYDROL.
      C     XWSEG     NUMBER OF WATER COLUMN SEGMENTS
      C     HENRY     HENRYS CONSTANT (SET TO ZERO TO SKIP
      C               VOLATILIZATION)                                UNITLESS
      C     MOLWT     MOLECULAR WEIGHT OF TOXICANT
      C     KLT       TEMPERATURE CORRECTION FACTOR FOR
      C               VOLATILIZATION
      C     ATMOS     CONCENTRATION OF TOXICANT IN THE
      C               ATMOSPHERE
      C     IFLOW     FLAG INDICATING A FLOWING ( 0.) OR
      C               A NON-FLOWING ( 1.) WATER BODY
      C     AI        MASS DEPENDENT ADSORPTION EXPONENT
      C               FOR SOLIDS TYPE I
      C     BI        MASS DEPENDENT ADSORPTION COEFFICIENT
      C               FOR SOLIDS TYPE I
      C     RHOI      DENSITY OF SOLIDS TYPE I                        GM/ML
      C
      C***********************************************************************
      C
      C
0011        DIMENSION PART(4),RHO(3),PARTOX(3),BIOS(3)
0012        EQUIVALENCE(TIME,T)
      C
      C
0013        REAL KD,KDT,KP,KPT,KD20,KP20,KHOH,KHOH20,KHN,KHN20,KHH,KHH20
0014        REAL KH,KHT,KL,KLA,KLT,MOLWT
      C
0015        EQUIVALENCE (CONST(1),KD20)
0016        EQUIVALENCE (CONST(2),KDT),(CONST(3),KP20),(CONST(4),KPT)
0017        EQUIVALENCE (CONST(5),KHOH20),(CONST(6),KHN20),(CONST(7),KHH20)
0018        EQUIVALENCE (CONST(8),KHT),(CONST(9),XWSEG),(CONST(10),HENRY)
0019        EQUIVALENCE (CONST(11),MOLWT),(CONST(12),KLT)
0020        EQUIVALENCE (CONST(13),ATMOS),(CONST(14),IFLOW),(CONST(15),AIRTMP)
0021        EQUIVALENCE (CONST(16),A1),(CONST(17),B1),(CONST(18),RHO1)
0022        EQUIVALENCE (CONST(19),A2),(CONST(20),B2),(CONST(21),RHO2)
0023        EQUIVALENCE (CONST(22),A3),(CONST(23),B3),(CONST(24),RHO3)
```

```
      C
0024          DIMENSION PH(75),TEMP(75),BACW(75),BACS1(75)
0025          DIMENSION BACS2(75),BACS3(75)
0026          DIMENSION DEPTH(75),TDEPTH(75),DWNSEG(75),AREA(75),WVEL(1)
      C
0027          EQUIVALENCE (PARAM(1,1),DEPTH(1)),(PARAM(1,2),TDEPTH(1))
0028          EQUIVALENCE (PARAM(1,3),DWNSEG(1)),(PARAM(1,4),AREA(1))
0029          EQUIVALENCE (PARAM(1,5),PH(1)),(PARAM(1,6),TEMP(1))
0030          EQUIVALENCE (PARAM(1,7),WVEL(1))
0031          EQUIVALENCE (PARAM(1,8),BACW(1)),(PARAM(1,9),BACS1(1))
0032          EQUIVALENCE (PARAM(1,10),BACS2(1)),(PARAM(1,11),BACS3(1))
      C
0033          COMMON /PHOTO/ DAYK(75)
      C
      C
      C           EVALUATE STRAIGHT LINE FUNCTIONS
      C
0034          IF(NFUNC.EQ.0) GOTO 4
0036          IF(NFUNT-T) 2,2,4
0037        2 IEV = 6
0038          IOPT = 2
0039          ITIME=ITIMF
0040          ITIMF = ITIMF + 1
0041          CALL WASP8
      C       SET DTIME
0042        4 DTIME = T-NFUNT
      C
      C
      C       DECIDE IF IT IS DUMPING TIME
      C
0043          IF(NDEVL-1.) 20,10,20
0044       10 IREC = IREC + 1
0045          IGOTO = 1
0046          NDEVL = 0.
0047          MXDMP = 3
0048          DUMMY = 0.0
0049          DO 13 I=1,NOSYS
0050  13      IRECL(I) = MXSEG*(IREC-1) + 1
0051          NUM = 10
0052          CALL FILEOC(NUM)
0053          WRITE(10'IREC)TIME
0054          GO TO 25
0055       20 IGOTO = 2
0056       25 CONTINUE
      C
0057          RHO(1) = RHO1
0058          RHO(2) = RHO2
0059          RHO(3) = RHO3
      C
      C          MOLECULAR DIFFUSIVITY (METERS**2/S)
      C
0060          DIFF = 22.E-09/(MOLWT**0.6666)
      C
      C          SET VISCOUS SUBLAYER AND DRAG COEFFICIENTS
      C
0061            XLAM2 = 4.
0062            CDRAG = 0.0011
      C
      C             SEGMENT LOOP
      C
0063            DO 100 I = 1,NOSEG
      C
0064            STP20 = TEMP(I) - 20.
      C
      C
      C         COMPUTE SEGMENT POROSITY
      C
0065            SLV = 0.0
0066            DO 26 J=2,NOSYS
0067         26 SLV = SLV + C(J,I)*1.E-06/RHO(J-1)
0068            PORE = 1. - SLV
      C
      C
      C********************************************************************
      C
      C         SYSTEM 1   TOXICANT
      C
      C********************************************************************
      C
      C
      C
      C         COMPUTE PARTICULATE AND DISSOLVED FRACTION FOR EACH SEGMENT
      C
0069            SUMMP = 0.0
      C
      C          CALCULATE PARTITION COEFFICIENTS
      C
      C
0070            PART(1) = 0.0
0071            IF(C(2,I).EQ.0.0) GO TO 501
0073            PART(2) = B1/(C(2,I)**A1)
0074        501 IF(NOSYS.GE.3.AND.C(3,I).GT.0.0) PART(3) = B2/(C(3,I)**A2)
0076            IF(NOSYS.GE.4.AND.C(4,I).GT.0.0) PART(4) = B3/(C(4,I)**A3)
      C
      C
      C
      C
0078            DO 30 J = 2,NOSYS
0079            IF(SYSEXC(J).EQ.1) GO TO 30
0081            SUMMP = SUMMP + C(J,I)*PART(J)
0082         30 CONTINUE
0083            FPART(1,I) = 1./(PORE+SUMMP)
0084            DISTOX = FPART(1,I)*C(1,I)
0085            DO 35 J = 2,NOSYS
0086            FPART(J,I) = C(J,I)*PART(J)/(PORE+SUMMP)
0087         35 PARTOX(J-1) = FPART(J,I)*C(1,I)
      C
      C
```

```
C
C
C        BIODEGRADATION :  SECOND ORDER KINETICS ASSUMED
C
      KD = KD20*(KDT**STP20)
      KP = KP20*(KPT**STP20)
C
C          A)  DEGRADATION IN WATER
C
      BIOW = KD*BACW(I)*DISTOX*PORE
C
C          B)  DEGRADATION ON SEDIMENT
C
      DO 40 J=2,NOSYS
      JJ = J-1
      IF(C(J,I).GT.0.)GO TO 39
      BIOS(JJ) = 0.0
      GO TO 40
   39 BIOS(JJ) = KP*BACS1(I)*PARTOX(JJ)*C(J,I)
   40 CONTINUE
C
C        HYDROLYSIS :  ALKALINE, NEUTRAL, AND ACID HYDROLYSIS CONSIDERED
C
C           COMPUTE HYDROGEN AND HYDROXIDE ION CONCENTRATION
C
      PPHI = PH(I)
      H = 1./(10.**PPHI)
      OH = 1.E-14/H
C
      XXX = KHT**(TEMP(I)-20.)
      KHOH = KHOH20*XXX
      KHN = KHN20*XXX
      KHH = KHH20*XXX
C
      KH = KHOH*OH + KHN + KHH*H
      HYDROL = KH*DISTOX*PORE
C
C       PHOTOLYSIS: DIRECT PHOTOLYSIS ONLY
C
      PHOTOL = DAYK(I)*DISTOX*PORE
C
C
C        VOLATILIZATION
C
      VOLAT = 0.0
      IF(HENRY.EQ.0.0) GO TO 47
      IF (TDEPTH(I).NE.0.0) GO TO 47
      IF (IFLOW.EQ.1) GOTO 45
      KK = 1
      QSCAL = SCALEQ(1,1)
      KMAX = FIELDQ(1)
      DO 931 K=1,KMAX
  931 IF(JQ(K).EQ.I.AND.IQ(K).EQ.DWNSEG(I)) GO TO 933
      WRITE(OUT,932) I
```

```
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0123   932    FORMAT(//'$$$$ ERROR IN SPECIFICATION OF DOWNSTREAM SEGMENT
            2 FOR SEGMENT',I4,' $$$$')
0124          CALL ABORT(28)
0125      933 GO TO (44,43,43),IQOPT
0126       43 KK=K
       C
       C      USE CONVERSION FACTOR 0.0864 TO CONVERT FLOW FROM
       C      10**6 CUBIC FEET/DAY  TO  CFS
       C
0127       44 Q = (MQ(KK)*(T-NQT) + BQ(K))*QSCAL/0.0864
       C
       C      CONVERSION FACTOR 0.3043 TO CONVERT VELOCITY FROM FPS
       C      TO METERS/S
       C
0128          VEL = (Q/AREA(I)) * 0.3048
0129          XKL = SQRT(DIFF*VEL/DEPTH(I)) * 86400.
0130          XKGH = 100.*HENRY
0131          KL = (1./(1./XKL + 1./XKGH)) * KLT**STP20
0132          GOTO 46
       C
       C      COMPUTE DENSITY (G/ML) AND VISCOSITY (M**2/S) OF AIR AND WATER
       C
0133       45 DENA = 0.001293/(1.+0.00367*AIRTMP)
0134          DENW = 1. - 8.8E-05*TEMP(I)
0135          XNUA = (1.32 + 0.009*AIRTMP) * 1.E-05
0136          XNUW = (10.**(1301./(998.333+8.1855*STP20+0.00585*STP20**2)-
            $ 3.30233)/DENW) * 1.E-04
0137          XKL = (DIFF/XNUW)**.666*SQRT(CDRAG*DENA/DENW)*.74*WVEL(I)/XLAM2
0138          XKG = (DIFF/XNUA)**.666*SQRT(CDRAG)*.74*WVEL(I)/(XLAM2)
0139          XKGH = XKG*HENRY
0140          KL = (1./(1./XKL + 1./XKGH)) * KLT**STP20*86400.
0141       46 KLA = KL/DEPTH(I)
0142          VOLAT = KLA * (DISTOX*PORE - ATMOS/HENRY)
0143       47 CONTINUE
       C
       C
       C      KINETIC DERIVATIVE
       C
0144          CD(1,I) = -(BIOW+BIOS(1)+BIOS(2)+BIOS(3)+HYDROL
            2 + PHOTOL + VOLAT)
       C
       C
       C      MULTIPLY BY VOLUME TO BE CONSISTANT WITH TRANSPORT CALCULATION
       C
0145          CD(1,I) = CD(1,I)*BVOL(I)
       C
       C
       C*********************************************************************
       C
       C      SYSTEM 2   SOLIDS
       C
       C*********************************************************************
       C
       C
```

```
C
C     NO KINETICS FOR SOLIDS SYSTEMS
C
C     CD(2,I) = 0.0
C
      CD(2,I) = 0.0
      CD(3,I)= 0.0
      CD(4,I)= 0.0
C
C
  100 CONTINUE
C
C     DUMP RESULTS TO DISK AT SPECIFIED INTERVALS
C
      IF(IGOTO .NE. 1) GO TO 951
      NUM = 11
      CALL FILEOC(NUM)
      DO 901 I=1,NOSEG
      IRC1=IRECL(1)
      DISTOX=C(1,I)*FPART(1,I)*1000.0
      PARTOX(1)=C(1,I)*FPART(2,I)*1000000.0/C(2,I)
      TOTTOX = C(1,I)*1000.
C
901   WRITE (11'IRC1) TOTTOX,DISTOX,PARTOX(1)
      NUM = 12
      CALL FILEOC(NUM)
      DO 902 I=1,NOSEG
      IRC2=IRECL(2)
C
  902 WRITE(12'IRC2)C(2,I),C(3,I),C(4,I)
  951 CONTINUE
C
      RETURN
      END
```

APPENDIX 3

Test Program Input and Output

To test that the computer code for the exposure concentration component of WASTOX is working correctly on the user's computer, a simple lake problem is provided. Two segments, representing the epilimnion and hypolimnion, are considered. An inflow and outflow of 1000 cfs occurs in the epilimniom. Settling occurs at a flow rate of 10 cfs. An exchange of 10^7 ft^3/d is inputted between the segments but is bypassed in the test run. The chemical enters at a concentration of 10 µg/ℓ (0.01 mg/ℓ). Adsorption, volatilization, and photolysis are considered.

INPUT

```
    1
    1    1    1    2    2
WASTOX TEST RUN EXAMPLE 1-B
TIME VARIABLE
00
    1    1                      ***** EXCHANGES *****
    1    2                      ***** WATER COLUMN DISPERSION *****
       0.0    1       0.0    2  ***** NO DISPERSION *****
       10.    1    2
*           1.0
                                                            SCALE FACTOR
    1    2                      ***** VOLUMES *****
1000.     2000.
*           1.0
                                                            SCALE FACTOR
    1    2                      ***** FLOWS *****
    2    2    0                 ***** HYDRONANMIC FLOW *****
       1.0    1       1.0    2
     1000.    1    0      1000.   0    1
*           1.0
                                                            SCALE FACTOR
    2    1    0                 ***** SETTLING OF SOLIDS *****
       1.0    2
       10.    2    1       10.    0    2
*           1.0
                                                            SCALE FACTOR
    1    1                      ***** BOUNDARY CONDITIONS *****
      0.01    1
*           1.0
                                                            SCALE FACTOR
    1    1
      100.    1
*      1.0
                                                            SCALE FACTOR
    1    0                      ***** NO FORCING FUNCTIONS *****
    1    0                      ***** NO FORCING FUNCTIONS *****
 DPTH 10.       TDPT 0.0       DSEG 0.0       AREA 10000.      PH 7.0
 TEMP 20.       WVEL 4.47      BACW           BCS1
 DPTH 20.       TDPT 10.       DSEG 0.0       AREA 20000.      PH 7.0
 TEMP 20.       WVEL           BACW           BCS1
 KD20            KDT 1.0       KP20            KPT 1.0       KHOH
  KHN            KHN            KHN 1.0       WSEG 2.0       HNRY 0.001
 MLWT 1000.      KLT 1.0       ATMS 0.0       IFLW 1.0       ATMP 20.
   A1 0.0         B1 1.0       RHO1 2.65
    0                           ***** NO TIME FUNCTION *****
    1                           ***** PHOTOLYSIS *****
   27
1589.     1673.     1710.     1677.     1575.     1410.     1279.     1215.
1193.     1195.     1175.      938.      571.      334.      336.      434.
 577.      770.      945.     1007.     1053.      932.      597.      261.
  80.       18.        4.
 0.01                           ***** QUATUM YIELD *****
40.       80.       1.          ***** LATITUDE LONGITUDE SEASON *****
0.0028    0.0028    0.0026    0.0025    0.0024    0.0023    0.0022    0.0021
0.0020    0.0019    0.0018    0.00152   0.00122   0.0010    0.00082   0.00069
0.00056   0.00043   0.00035   0.0003    0.00026   0.00023   0.0002    0.00017
0.00016   0.00016   0.00016
0.0       1.0
 TOX  0.0       TOX  0.0        ***** INITIAL CONDITIONS OF TOXICANT *****
 SLD1 100.      SLD1 100.       ***** INITIAL CONDITIONS *****
10000.    10000.                ***** STABILITY CRITERIA *****
15.                             ***** PRINT INTERVAL *****
0.1       360.                  ***** TIME STEP, TOTAL TIME *****
TOT TOX DISSTOX PARTOX
  1  1  2
  2  1  2
  3  1  2

SOLIDS
  1  1  2
```

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OUTPUT

```
                              MODEL  1 SERIES  1 RUN  1

   WASTOX TEST RUN EXAMPLE 1-B
                                      2 SEGMENT    2 SYSTEM MODEL


 SYSTEMS SELECTED FOR PROCESSING---
                                         1
                                         2

                                     EXCHANGE COEFFICIENTS-R(1.E+06 CF/D)

                                 R OPTION  1 USED     NO. OF R FIELDS    1


 FIELD  1               ***** WATER COLUMN DISPERSION *****
 ---------

   SYSTEM  SCALE  FACT  SYSTEM  SCALE  FACT  SYSTEM  SCALE, FACT  SYSTEM  SCALE  FACT  SYSTEM  SCALE  FACT
      1    0.0000E+00      2    0.0000E+00

 SCALE FACTOR IS [*  1.0000000       UNITS ARE --                    ]
 THE ADJUSTED VALUES ARE --


R    TO FROM

  0.100E+02    1    2

                                         VOLUMES-VOL(1.E+06 CF)

                                 VOL OPTION  1 USED    NO. OF VOLS READ    2


 SCALE FACTOR IS [*  1.0000000       UNITS ARE --                    ]
 THE ADJUSTED VALUES ARE --

     VOL       VOL       VOL       VOL       VOL       VOL       VOL       VOL

  0.100E+04 0.200E+04
```

```
                              FLOWS=Q(CFS)

            FLOW OPTION  1 USED     NO. OF FLOW FIELDS    2


FIELD  1                ***** HYDRODANNIC FLOW *****
---------

  SYSTEM  SCALE FACT  SYSTEM  SCALE FACT  SYSTEM  SCALE FACT  SYSTEM  SCALE FACT  SYSTEM  SCALE FACT
     1    0.1000E+01     2    0.1000E+01

SCALE FACTOR IS [*  1.0000000        UNITS ARE --                    ]
THE ADJUSTED VALUES ARE --

     FLOW     TO  FROM     FLOW     TO  FROM     FLOW     TO  FROM     FLOW     TO  FROM

 0.100E+04     1     0 0.100E+04     0     1

FIELD  2                ***** SETTLING OF SOLIDS *****
---------

  SYSTEM  SCALE FACT  SYSTEM  SCALE FACT  SYSTEM  SCALE FACT  SYSTEM  SCALE FACT  SYSTEM  SCALE FACT
     2    0.1000E+01

SCALE FACTOR IS [*  1.0000000        UNITS ARE --                    ]
THE ADJUSTED VALUES ARE --

     FLOW     TO  FROM     FLOW     TO  FROM     FLOW     TO  FROM     FLOW     TO  FROM

 0.100E+02     2     1 0.100E+02     0     2
```

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```
                              BOUNDARY CONCENTRATIONS FOR SYSTEM  1
                            BC OPTION  1 USED      NO.OF BC"S READ    1


        SCALE FACTOR IS [*  1.0000000        UNITS ARE --                       ]
        THE ADJUSTED VALUES ARE --

          BC  SEG         BC  SEG         BC  SEG         BC  SEG         BC  SEG         BC  SEG

      0.1000E-01   1

                              BOUNDARY CONCENTRATIONS FOR SYSTEM  2
                            BC OPTION  1 USED      NO.OF BC"S READ    1


        SCALE FACTOR IS [*  1.0000000        UNITS ARE --                       ]
        THE ADJUSTED VALUES ARE --

          BC  SEG         BC  SEG         BC  SEG         BC  SEG         BC  SEG         BC  SEG

      0.1000E+03   1

                              FORCING FUNCTIONS FOR SYSTEM  1    (LBS/DAY)


                              FORCING FUNCTIONS FOR SYSTEM  2    (LBS/DAY)


                             SEGMENT PARAMETERS FOR SEGMENT  1

         DPTH=  0.10000E+02  TDPT=  0.00000E+00  DSEG=  0.00000E+00  AREA=  0.10000E+05    PH=  0.70000E+01
         TEMP=  0.20000E+02  WVEL=  0.44700E+01  BAC=   0.00000E+00  BCS1=  0.00000E+00

                             SEGMENT PARAMETERS FOR SEGMENT  2

         DPTH=  0.20000E+02  TDPT=  0.10000E+02  DSEG=  0.00000E+00  AREA=  0.20000E+05    PH=  0.70000E+01
         TEMP=  0.20000E+02  WVEL=  0.00000E+00  BAC=   0.00000E+00  BCS1=  0.00000E+00

                                      CONSTANTS

                                                                      KPT=  0.10000E+01  KHOH=  0.00000E+00
      KD20=  0.00000E+00   KDT=  0.10000E+01  KP20=  0.00000E+00    WSEG=  0.20000E+01  HNRY=  0.10000E-02
       KHN=  0.00000E+00   KHN=  0.00000E+00   KHN=  0.10000E+01    IFLW=  0.10000E+01  ATMP=  0.20000E+02
      MLWT=  0.10000E+04   KLT=  0.10000E+01  ATMS=  0.00000E+00
        A1=  0.00000E+00    B1=  0.10000E+01  RHO1=  0.26500E+01
```

```
                    P H O T O L Y S I S

LATITUDE 40. DEGREES      LONGITUDE 80. DEGREES       SEASON 1.

WAVELENGTH     MOLAR EXTINCTION (L/MOLE-CM)    IRRADIANCE DECAY RATE (1/METER)

   297.5             0.1589E+04                      0.2800E-02
   300.0             0.1673E+04                      0.2800E-02
   302.5             0.1710E+04                      0.2600E-02
   305.0             0.1677E+04                      0.2500E-02
   307.5             0.1575E+04                      0.2400E-02
   310.0             0.1410E+04                      0.2300E-02
   312.5             0.1279E+04                      0.2200E-02
   315.0             0.1215E+04                      0.2100E-02
   317.5             0.1193E+04                      0.2000E-02
   320.0             0.1195E+04                      0.1900E-02
   323.1             0.1175E+04                      0.1800E-02
   330.0             0.9380E+03                      0.1520E-02
   340.0             0.5710E+03                      0.1220E-02
   350.0             0.3340E+03                      0.1000E-02
   360.0             0.3360E+03                      0.8200E-03
   370.0             0.4340E+03                      0.6900E-03
   380.0             0.5770E+03                      0.5600E-03
   390.0             0.7700E+03                      0.4300E-03
   400.0             0.9450E+03                      0.3500E-03
   410.0             0.1007E+04                      0.3000E-03
   420.0             0.1053E+04                      0.2600E-03
   430.0             0.9320E+03                      0.2300E-03
   440.0             0.5970E+03                      0.2000E-03
   450.0             0.2610E+03                      0.1700E-03
   460.0             0.8000E+02                      0.1600E-03
   470.0             0.1800E+02                      0.1600E-03
   480.0             0.4000E+01                      0.1600E-03

    FRACTION OF SKY CLOUDY0.000     LIGHT REDUCTION FACTOR  0.1000E+01
```

```
                              INITIAL CONDITIONS

*******************************************************************************

                                 ***********
                                 * SYSTEM  1 *
                                 ***********

       NAME    CONC.      NAME    CONC.      NAME    CONC.     NAME    CONC.
       ------ --------   ------ --------   ------ --------   ------ --------
       TOX   0.0000E+00  TOX   0.0000E+00

                                 ***********
                                 * SYSTEM  2 *
                                 ***********

       NAME    CONC.      NAME    CONC.      NAME    CONC.     NAME    CONC.
       ------ --------   ------ --------   ------ --------   ------ --------
       SLD1  0.1000E+03  SLD1  0.1000E+03


              STABILITY AND ACCURACY CRITERIA FOR NUMERICAL INTEGRATION

*******************************************************************************

                 SYSTEM   MAXIMUM CONCENTRATION
                 -------- ----------------------

                    1            10000.00

                    2            10000.00

    PRINT INTERVAL     15.00

    INTEGRATION INTERVAL     0.1000
    TOTAL TIME  360.0000
```

```
                              DUMPS FROM SYSTEM  1

TIME        1           2              1           2              1           2
         TOT TOX      TOT TOX       DISSTOX     DISSTOX         PARTOX      PARTOX
   0.0  0.0000E+00  0.0000E+00    0.0000E+00  0.0000E+00     0.0000E+00  0.0000E+00
  15.0  0.4554E+01  0.1303E-01    0.4541E-01  0.1290E-03     0.4541E+02  0.1290E+00
  30.0  0.4862E+01  0.2111E-01    0.4858E-01  0.2090E-03     0.4858E+02  0.2090E+00
  45.0  0.4881E+01  0.2366E-01    0.4880E-01  0.2343E-03     0.4880E+02  0.2343E+00
  60.0  0.4882E+01  0.2439E-01    0.4881E-01  0.2415E-03     0.4881E+02  0.2415E+00
  75.0  0.4882E+01  0.2459E-01    0.4881E-01  0.2435E-03     0.4881E+02  0.2435E+00
  90.0  0.4882E+01  0.2465E-01    0.4881E-01  0.2441E-03     0.4881E+02  0.2441E+00
 105.0  0.4882E+01  0.2466E-01    0.4881E-01  0.2442E-03     0.4881E+02  0.2442E+00
 120.0  0.4882E+01  0.2466E-01    0.4881E-01  0.2443E-03     0.4881E+02  0.2443E+00
 135.0  0.4882E+01  0.2466E-01    0.4881E-01  0.2443E-03     0.4881E+02  0.2443E+00
 150.0  0.4882E+01  0.2466E-01    0.4881E-01  0.2443E-03     0.4881E+02  0.2443E+00
 165.0  0.4882E+01  0.2466E-01    0.4881E-01  0.2443E-03     0.4881E+02  0.2443E+00
 180.0  0.4882E+01  0.2466E-01    0.4881E-01  0.2443E-03     0.4881E+02  0.2443E+00
 195.0  0.4882E+01  0.2466E-01    0.4881E-01  0.2443E-03     0.4881E+02  0.2443E+00
 210.0  0.4882E+01  0.2466E-01    0.4881E-01  0.2443E-03     0.4881E+02  0.2443E+00
 225.0  0.4882E+01  0.2465E-01    0.4881E-01  0.2443E-03     0.4881E+02  0.2443E+00
 240.0  0.4882E+01  0.2465E-01    0.4881E-01  0.2443E-03     0.4881E+02  0.2443E+00
 255.0  0.4882E+01  0.2465E-01    0.4881E-01  0.2443E-03     0.4881E+02  0.2443E+00
 270.0  0.4882E+01  0.2465E-01    0.4881E-01  0.2443E-03     0.4881E+02  0.2443E+00
 285.0  0.4882E+01  0.2465E-01    0.4881E-01  0.2443E-03     0.4881E+02  0.2443E+00
 300.0  0.4882E+01  0.2465E-01    0.4881E-01  0.2443E-03     0.4881E+02  0.2443E+00
 315.0  0.4882E+01  0.2465E-01    0.4881E-01  0.2443E-03     0.4881E+02  0.2443E+00
 330.0  0.4882E+01  0.2465E-01    0.4881E-01  0.2443E-03     0.4881E+02  0.2443E+00
 345.0  0.4882E+01  0.2464E-01    0.4881E-01  0.2443E-03     0.4881E+02  0.2443E+00
 360.0  0.4882E+01  0.2464E-01    0.4881E-01  0.2443E-03     0.4881E+02  0.2443E+00
```

```
                 DUMPS FROM SYSTEM  2

        TIME          1              2
                   SOLIDS         SOLIDS
         0.0   0.1000E+03     0.1000E+03
        15.0   0.9928E+02     0.1000E+03
        30.0   0.9908E+02     0.9999E+02
        45.0   0.9903E+02     0.9999E+02
        60.0   0.9902E+02     0.9998E+02
        75.0   0.9901E+02     0.9997E+02
        90.0   0.9901E+02     0.9997E+02
       105.0   0.9901E+02     0.9996E+02
       120.0   0.9901E+02     0.9996E+02
       135.0   0.9901E+02     0.9995E+02
       150.0   0.9901E+02     0.9995E+02
       165.0   0.9901E+02     0.9994E+02
       180.0   0.9901E+02     0.9993E+02
       195.0   0.9901E+02     0.9993E+02
       210.0   0.9901E+02     0.9992E+02
       225.0   0.9901E+02     0.9992E+02
       240.0   0.9901E+02     0.9991E+02
       255.0   0.9901E+02     0.9991E+02
       270.0   0.9901E+02     0.9990E+02
       285.0   0.9901E+02     0.9989E+02
       300.0   0.9901E+02     0.9989E+02
       315.0   0.9901E+02     0.9988E+02
       330.0   0.9901E+02     0.9988E+02
       345.0   0.9901E+02     0.9987E+02
       360.0   0.9901E+02     0.9987E+02
```